

# Linking Process, Structure, and Property in Additive Manufacturing Applications through Advanced Materials Modelling

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**Abstract:** Additive manufacturing (AM) processes have the ability to build complex geometries from a wide variety of materials. A popular approach for metal-based AM processes involves the deposition of material particles on a substrate followed by fusion of those particles together using a high intensity heat source, e.g. a laser or an electron beam, in order to fabricate a solid part. These methods are of high priority in engineering research, especially in applications for the energy, health, and defense sectors. The primary reasons behind the rapid growth in interest for AM include: (1) the ability to create complex geometries that are otherwise cost-prohibitive or difficult to manufacture, (2) increased freedom of material composition design through the adjustment of the elemental ratios of the composing powders, (3) a reduction in wasted materials, and (4) fast, low-volume, production of prototype and functional parts without the additional tooling and die requirements of conventional manufacturing methods. However, the highly localized and intense nature of these processes elicits many experimental and computational challenges. These challenges motivate a strong need for computational investigation, as does the need to more accurately characterize the response of parts built using AM. The present work will discuss these challenges and methods for creating multiscale material models that account for the complex phenomena observed in additively manufactured products. The linkage between process, structure, and property of AM components, e.g., anisotropic plastic behavior combined with anisotropic microstructural descriptors afforded through enhanced data compression techniques, will also be discussed.

## 1 INTRODUCTION

Additive manufacturing (AM) is a set of processing methods that can be used for developing 3D products incrementally in a layer-by-layer fashion. AM for metallic components has risen to be one of the major research thrusts in materials science and engineering over the past decade. The highest impact of metal-based AM has been felt in areas of advanced manufacturing, mechanical engineering, materials science, aerospace engineering, and bio-medical engineering. These processes have an impressive potential for impact in many government and industry sectors while also having positive societal and entrepreneurial effects. Future applications of AM include the possibility for many opportunities in coupled process-structure-property-product design. AM is nearly limitless in its ability to create complex geometric features, unlike subtractive processes, such that topological design and metamaterial design is only constrained by the product functionality instead of manufacturability. Unique powder combinations and process parameter flexibility yield the possibility for functionally graded materials and localized microstructure/property design. Materials design is also a natural consequence of AM using powder metallurgy in order to adjust bulk material composition.

While processes falling under the umbrella of metal-based AM have created a foundation which has the potential to revolutionize advanced manufacturing and design, as-built AM materials are not well understood and the relationship between the AM process parameters and the resulting structural properties remain unknown. The present work provides a comprehensive view of AM for alloy powder fusion from the standpoints of materials science and engineering with applications of advanced material modeling used to determine process-structure-property relations. A brief explanation of the various AM processes are given in Section 2 followed by experimental materials characterization in Section 3. Microstructure descriptor data compression techniques are discussed in Section 4. The current approaches taken by the authors in 3D image-based constitutive modeling based on 3D microstructure reconstruction of microstructure defects in as-built AM alloys are demonstrated in Section 5. Methods for new advanced model development are described in Section 6 followed by concluding remarks in Section 7.

## **2 METAL-BASED AM PROCESSES**

There are two primary components that can be used to differentiate between metal-based AM fusion processes: (1) powder accumulation and (2) energy input. Accumulation is the method of placing the powder particles in front of the energy input for subsequent fusion while the method of energy input is the physical process that is used to transfer energy into the particles in order to cause a phase change. The chosen combination of these components can drastically affect material performance.

### **2.1 Accumulation Methods**

The primary methods for accumulation of powder material in front of the energy source include direct deposition, e.g., Laser Engineered Net Shaping (LENS), an active process, and powder-bedding, e.g., Selective Laser Melting (SLM) and Electron Beam Melting (EBM), a passive process. Direct deposition simply means that a spray system is utilized in order to direct the powder material into the focal point of the energy source. This method is excellent for manufacturing free-form structures and for component repair. Direct deposition typically has a low amount of wasted powder because the deposition is local. This method also requires 3D control of the tooling used for energy input and powder spray. Powder-bedding is the process of spreading a thin layer of powder which is selectively melted to create contour of the desired geometry. Successive layers will accumulate until the final product is formed. This method is not as versatile in terms of controllability for applications such as component repair because only 2D control is necessary (the powder bed is generally moved vertically downward after each layer is completed such that the new layer can be deposited).

### **2.2 Energy Input Methods**

Energy inputs used in metal-based AM include lasers and electron beams. Laser-based additive manufacturing uses a mobile laser head. The laser beam is capable of emitting photons to a focal point located on a substrate and the collision of these photons with the surface produce enough heat to change the phase of the substrate. State-of-the-art laser technology allows numerous control methods including modulation and pulsing, fine-scale adjustments to spot diameter and a wide range of power output settings. Electron-based additive manufacturing uses a mobile electron beam in order to create the 2D planar sections but using much different physical mechanisms than laser-based methods. The electron beam, as the name implies, emits electrons to a focal point on the substrate which penetrate the material; the kinetic energy of these electrons is transformed into heat upon contact with the substrate.

### **2.3 Computational Process Modeling for AM Processes**

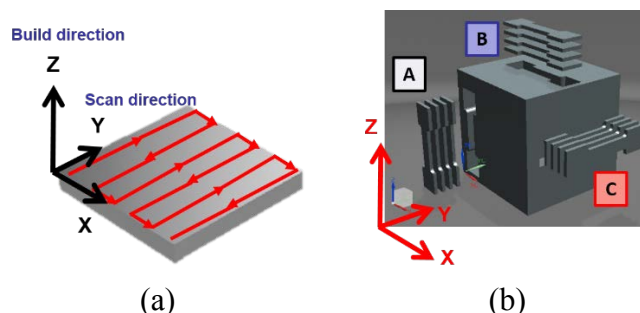
Process modeling for AM can play a pivotal role in understanding the complex mechanics of AM processes while predicting the microstructural properties of AM products, the thermal

history, and the cooling rates for a given set of process parameters. While the many computational complexities related to the multi-physics and multi-scale nature of AM process modeling are beyond the scope of the present study, mention should be made of the primary differences that arise due to the choice of accumulation and energy input methods. The modeling of the energy input is of ample importance in predicting the physical processes that take place during AM processing. Because the physics utilized for laser-based and electron beam-based processing are different, using a heat source model (energy input model) based on the physics of electron beam-based processing [1] for simulation of laser-based processing would yield unphysical results.

The effect of the accumulation method on process modeling is in the material microstructure and properties. In direct deposition, the powder is typically melted as soon as it hits the substrate, which is in a liquid, solid, or mushy state but is not in powder form, and therefore the thermal material properties of the powder is not likely to require consideration in the thermal response. Processes that incorporate a powder bed, however, will inherently require spatially and temporally varying material properties, based on the scanning strategy, to account for differences in the properties, e.g., absorptivity and thermal conductivity, of powder material as opposed to bulk material.

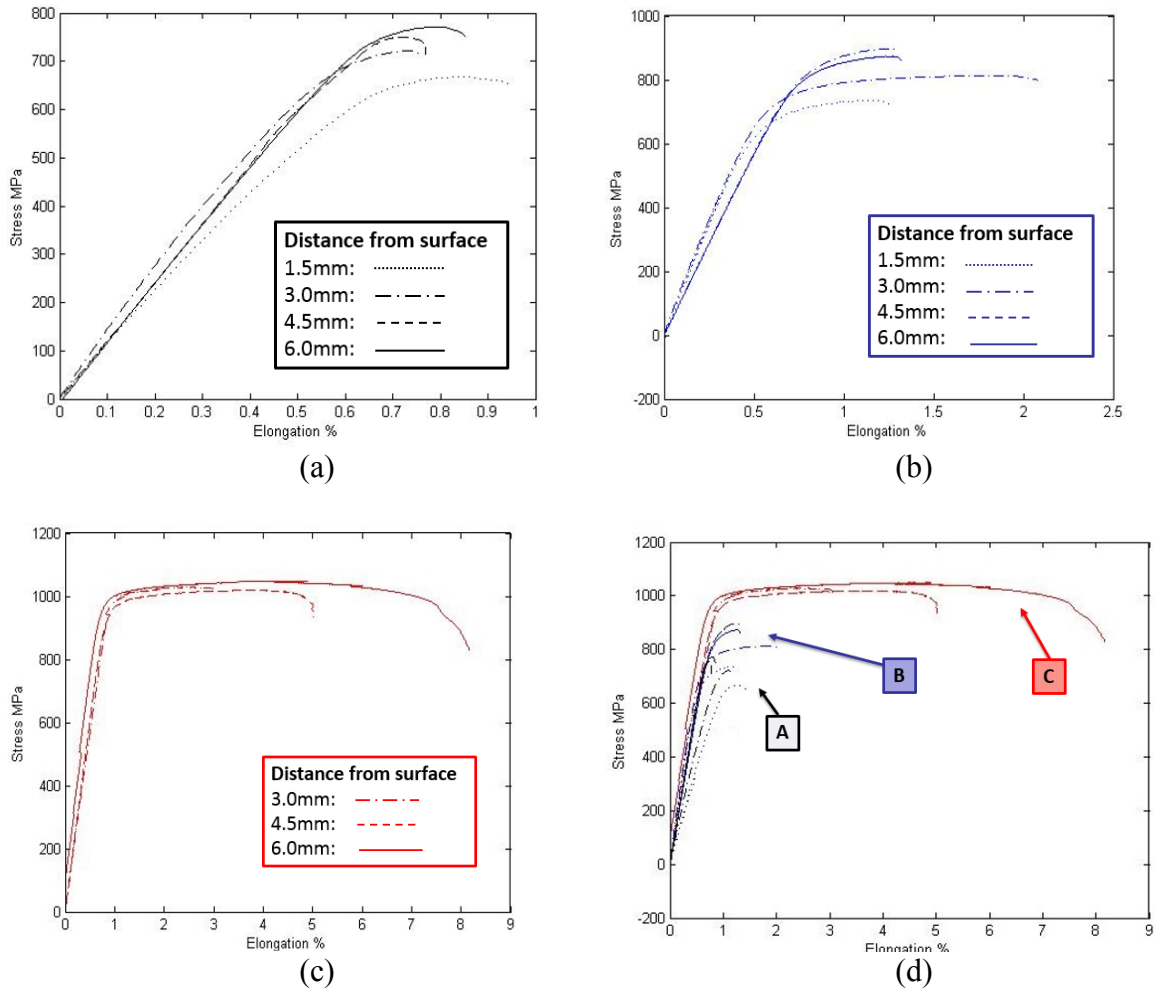
### 3 EXPERIMENTAL MATERIALS CHARACTERIZATION

Experimental characterization of AM products is critical in understanding the process-structure-property relationship. While products created using traditional manufacturing processes, e.g., metal forming and cutting, typically provide repeatable and low variations in the resulting material characterization, the highly localized and intense nature of AM processes result in a grand challenge for uncertainty quantification and management. Rapid changes in material properties are observed with only small changes in process parameters due to inhomogeneous and anisotropic microstructure. Figure 1 shows a schematic of a Ti-6Al-4V block of material to be manufactured using AM with all process parameters fixed with the exception of the scanning direction. The block was created and subsequently dissected in order to obtain tensile coupons in multiple orientations.



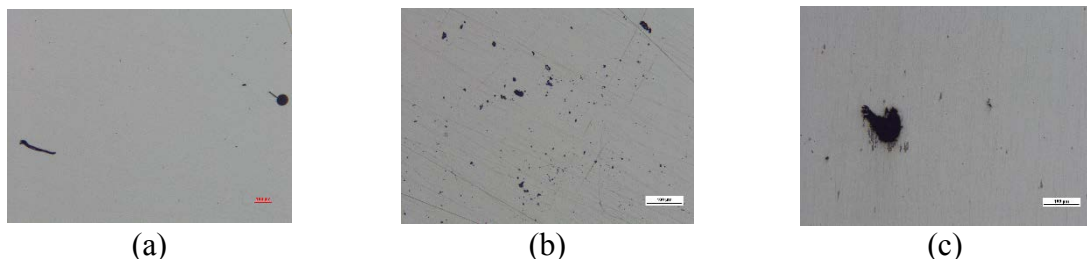
**Figure 1.** (a) Toolpath of Ti-6Al-4V build. Y denotes the scanning direction and Z denotes the build direction of the laser optic. (b) Schematic of manufactured cube for tensile specimen extraction in three orientations [2]

The stress-strain diagrams from the coupon specimens, corresponding to those shown in Figure 1, recovered from a block of Ti-6Al-4V alloy manufactured using the LENS process can be seen in Figure 2. It is clear that the mechanical behavior is strongly anisotropic in the elastic properties, plastic yield behavior, hardening behavior, damage evolution, and failure strain. These results are dictated completely by the scanning direction (Figure 1. (a)) and the distance from the free surface of the object, which causes the directional solidification of the microstructure. However, the impact of the microstructure on the anisotropic properties observed in Figure 2 are not intuitive and therefore must be investigated.



**Figure 2.** Uniaxial tensile test stress-strain curves for Ti-6Al-4V specimens for each orientation (see Figure 1) from surface to core; orientations (a) A, (b) B, (c) C, and (d) all curves [2]

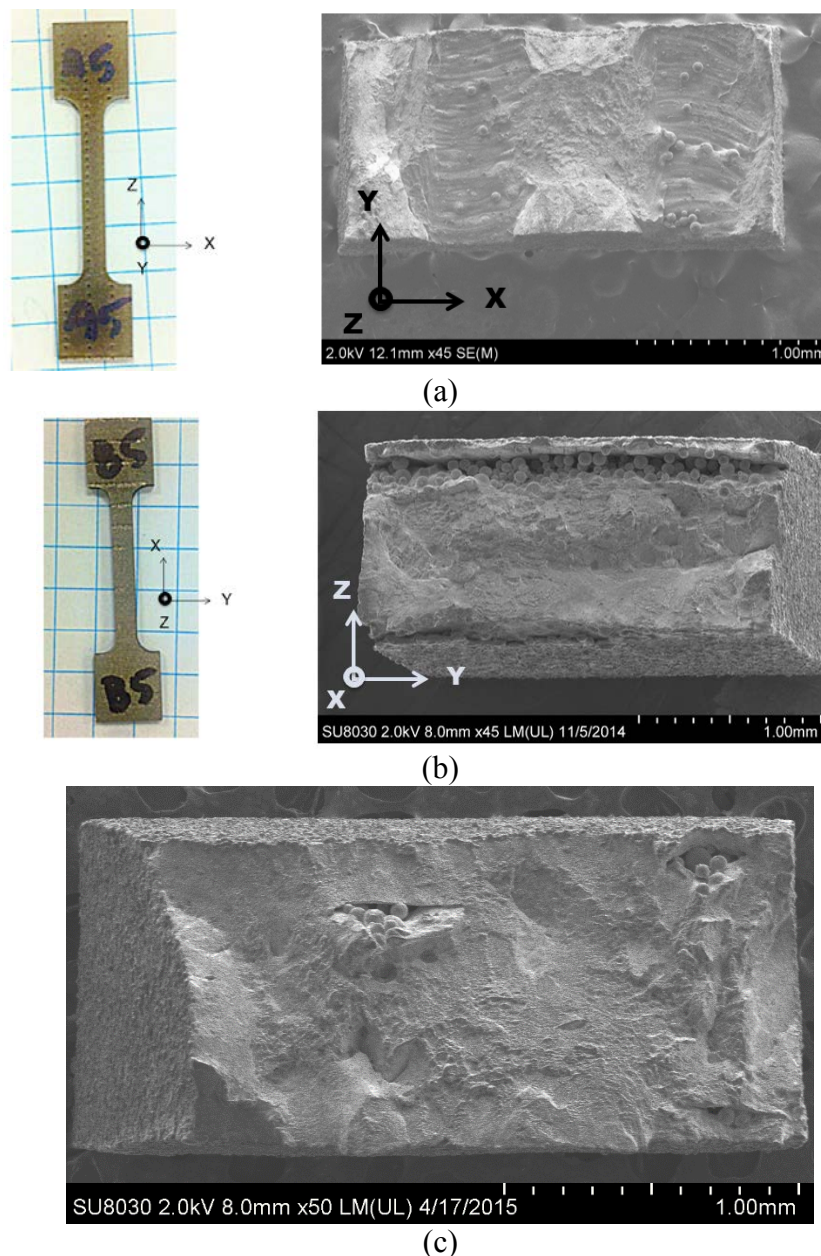
Figure 3 shows features of voids in an as-built alloy at various locations along a tensile coupon captured using optical microscopy images. A high level of porosity is clearly visible on the surface at all locations with the size of the voids ranging dramatically for each location. The highest amount of porosity is, not surprisingly, very close to the fracture surface of the tensile specimen while then ends have a lower overall distribution of voids. It can be easily understood that this is closely related to the laser energy input and thermal history during processing in the specific location of the sample.



**Figure 3.** Optical microscopy of voids observed at the (a) bottom, (b) near the fracture and at the (c) top [3] (scale bars are 100µm)

Figure 4 shows a close-up view of the fracture surface for the different orientations of tensile coupon made from the Ti-6Al-4V cube. The anisotropy in the microstructure can be seen in all images. A few notable characteristics of the microstructure at the fracture surface are: (1) large number of unmelted, or poorly melted, particles causing a high density of inclusions and

voids, (2) low success of interlayer bonding, and (3) multi-modal fracture behavior at the fracture site. Optimization of the laser processing parameters should be performed to improve properties of the current as-built alloys.



**Figure 4.** Surface porosity and fracture surfaces of Ti-6Al-4V samples after tensile testing for orientations (a) A, (b) B and (c) C (orientations are marked in Figure 1) [2].

A summary of the anisotropic nature of the coupon samples can be seen in Table 1. As can be seen in the table, the tensile coupon obtained from orientation C shows the highest ductility and strength while orientation A has the lowest ductility and strength. This indicates that the preferential direction in AM is in the laser scan direction. Comparing this result with the microstructural images shown in Figure 4 explains just how much microstructural conformation can play a role in the overall material performance of AM products. Unlike with traditional manufacturing processes, for which the material properties of the product are dictated primarily by the material composition, the material properties of AM materials has a dramatic impact from the microstructure.



**Table 1.** Average material properties for each orientation indicated in Figure 1 [2]

Orientation	Ultimate Tensile Strength (MPa)	Elongation at Fracture (%)	Modulus of Elasticity (GPa)	Bulk Porosity (%)
A	650	0.9	116	2.2
B	830	1.7	109	2.7
C	1012	6.0	144	2.0

The primary purpose of this section is to motivate the succeeding discussion on the development and implementation of advanced material modeling methods for AM products. Complex anisotropic material behavior and microstructures in AM products are quite unique compared to compositionally similar products developed using other manufacturing methods. Elucidating the relationship between processing, microstructure, properties, and product performance is perhaps the most important aspect in formulating materials and manufacturing design strategies for AM processes. While the tasks charged to the computational community are many, the present work indicates that advancements in computational methods for materials modeling has become an excellent alternative to pure experimental and data-driven methods in understanding process-structure-property relations in AM products.

#### **4 REDUCED ORDER MICROSTRUCTURAL MODELING USING ENHANCED DATA COMPRESSION**

A continuing challenge in computational modeling of heterogeneous materials is the prediction of macroscopic behavior from the material properties of each of its micro-constituents and the microstructure conformation in both an accurate and efficient manner. Particularly, the microstructure of the material plays an important role since microscale interactions between constituents has a strong contribution to the macroscale material properties. Due to the incremental nature of AM processes, the microstructure in the material of a product is quite complex and depends strongly on the processing parameters. On the other hand, as a primary interest of AM, specific microstructures, e.g., anisotropic material properties and microstructure conformation, can be controlled through careful process design strategies. The ability to develop modeling methodologies that can capture the effects of the microstructure in heterogeneous materials becomes even more desirable for applications in AM.

The most accurate method for linking the complex microstructure to the material properties is to perform direct numerical simulations (DNS), e.g., Finite Element Method (FEM) [4] and Fast Fourier Transform (FFT)-based micromechanics[5]. However, the high computational cost prohibits DNS methods from a multi-scale perspective as the microscopic simulation will be recomputed at each material point in the macroscopic simulation. Therefore, several reduced order methods have been proposed to improve the efficiency of the prediction without losing substantial accuracy. The first category of such methods is the micromechanics method, such as the Mori-Tanaka method for regularly shaped inclusions [6, 7] and the volume-integral based methods for arbitrarily shaped inclusions [8]. Although the micromechanics methods have been extensively applied to elastic materials, it is well understood that they have difficulties capturing localized nonlinear behavior such as plasticity and damage. More general methods have been developed to overcome the limitations of traditional micromechanics methods. In particular, intensive research has been focused on two approaches: (1) non-uniform transformation field analysis (NTFA) [9, 10] and (2) variants of the proper orthogonal decomposition (POD) [11]. For both approaches, the predictions under a loading condition are obtained by linear combination of a finite number of RVE modes from

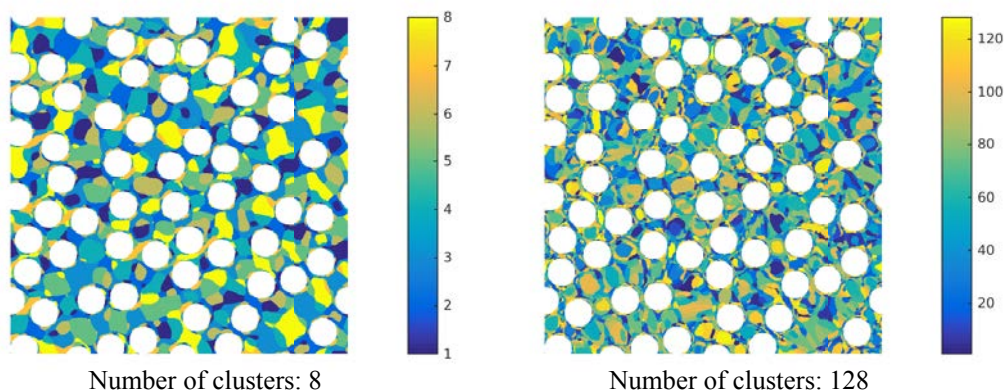
previously completed simulations under various load conditions. Due to limitations of the linear combination, extra efforts are required when dealing with nonlinear materials. For NTFA, specific evolution laws of internal variables have to be assumed for each mode. While for POD-based methods, excessive simulations are needed *a priori* in order to guarantee the robustness of the prediction under arbitrary loading conditions.

The proposed approach is developed to efficiently extract information from the microstructure through *a priori* calculation and utilizing the data in an efficient manner. This is made possible through incorporation of recently developed data compression algorithms, which greatly reduce the number of degree-of-freedom (DOF) in a calculation by finding the similarities in the data set. Based on the data compression and micromechanics-based clustering analysis, both microscopic and macroscopic nonlinear behaviors can be calculated rapidly and accurately. The approach can be easily applied to multi-scale constitutive modeling of AM products with complex material microstructures and properties.

As a primary step, the data set is obtained by *a priori* FEM simulations; each element in the FEM simulation generates one data point. In our work, the data type is defined by, but not restricted to, the strain concentration tensor  $\mathbf{A}(\mathbf{x})$  which relates the microscopic strain  $\boldsymbol{\varepsilon}_{micro}(\mathbf{x})$  to the macroscopic strain  $\boldsymbol{\varepsilon}_{macro}$ ,

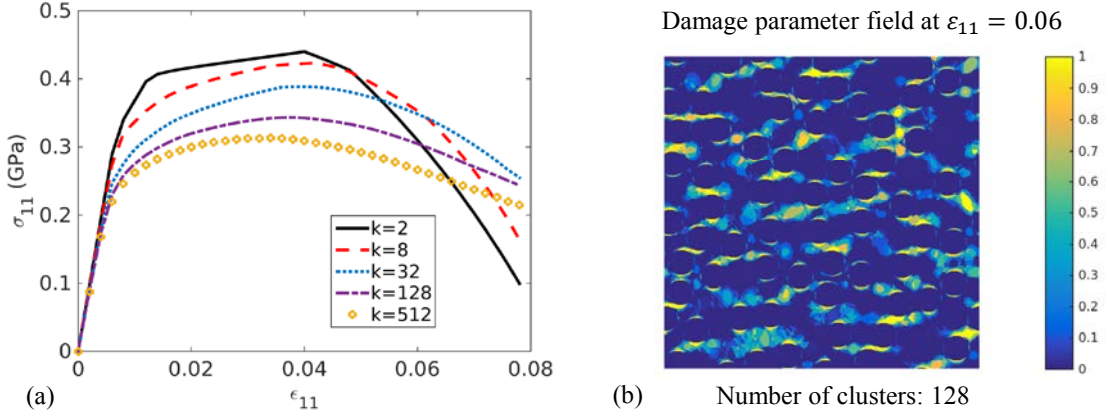
$$\boldsymbol{\varepsilon}_{micro}(\mathbf{x}) = \mathbf{A}(\mathbf{x}) : \boldsymbol{\varepsilon}_{macro}. \quad (1)$$

By definition, the similarity between two data points is characterized by the distance between the strain concentration tensor. As a well-studied data compression approach, clustering has been widely applied to pattern recognition, image analysis and bioinformatics. Clustering is used to group the data set in such a way that the data points in the same group are more similar to each other than to those in other groups. Two clustering results of a 2-dimensional (2D) porous material with different numbers of clusters are provided in Figure 6. This data compression approach in general can be applied to materials with arbitrary microstructures as long as the geometry is well resolved in the original DNS discretization.



**Figure 6.** Clustering results of a 2D porous material based on strain concentration tensors. The mesh size of the original FEM calculation is  $600 \times 600$ .

After the clustering step, a micromechanics-based clustering analysis is developed to compute the interaction tensors between clusters. Since the data points in one cluster are specified to have similar elastic behavior, it can be further assumed that there are uniform fields of internal variables in each cluster. With the help of Green's function, the original partial differential equilibrium equations can be rewritten in an integral form, and the plastic strain is naturally introduced into the integral equation as an eigenstrain term. By integrating the Green's function in each cluster, the interaction tensors can be obtained. Only a one-time calculation is required in order to obtain the interaction tensors; they can then be used for complex material behaviors without any modification.



**Figure 7.** (a) Uniaxial tensile simulated stress-strain curve for a 2D plastic porous material including damage, with number of clusters ranging from 2 to 512; (b) the field of damage parameter  $D$  at  $\epsilon_{11} = 0.06$  when number of clusters  $k = 128$ .  $D = 1$  indicates the material is fully damaged.

As an illustration, the clustering analysis is applied to a 2D plastic porous material with damage. As we can see from Figure 7, the stress-strain curves converge according to the number of clusters. The field of damage parameters can be well reproduced with only 128 DOFs, while the original FEM calculation has 360000 DOFs. In this sense, the computation cost is greatly reduced without losing the microscopic information. For AM material, the reduced order microstructural modelling based on advanced data compression provides an efficient and accurate tool for the following image-based constitutive modelling.

## 5 IMAGE-BASED MECHANISTIC PLASTICITY FOR AM MATERIALS

This section aims to explore the relationship between structure and performance of additively manufactured metals. The link between microstructure and macroscale material behavior is codependent. Global phenomena such as damage, fatigue, and fracture are dependent on microstructure features, which include crystallographic defects, voids, inclusions, allotropic phases, and crystal structures, e.g., secondary dendrite arms. Likewise, during a component's life cycle, microstructure will continue to evolve as a function of the local mechanical state. In order to accurately predict material behavior during the mechanical simulation of a component, the material model must be embedded with the correct microstructural descriptors. Unlike traditionally-manufactured metals, the microstructure of additively manufactured metals are highly variable within a single part, so these descriptors are expected to vary as a function of position within the part.

The benefits to using experimentally-informed microstructure reconstruction techniques are the following: (1) incorporating experimental data is more accurate than previous assumptions of homogeneous or periodic distributions; (2) it promotes the development of physically-motivated models, since parameters related to the microstructure are determined by experiment; and (3) more general constitutive relationships can be developed while allowing local microstructural information to account for anisotropy or heterogeneity. In this fashion, a single material model can be used to predict the mechanical response of a component's global behavior, and a standardized model may be developed for components generated from similar material compositions or manufacturing conditions. A more in-depth discussion of constitutive law development can be found in Section 6 of this paper.

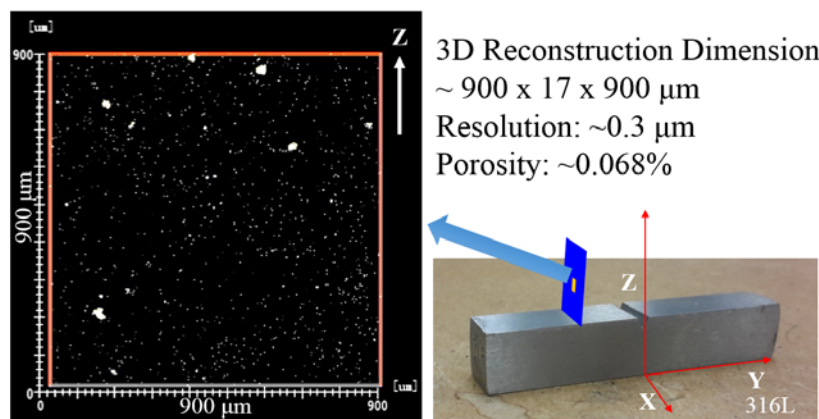
One natural approach to capturing microstructure information is through the use of image-based techniques. Once combined with the appropriate constitutive and evolution equations, the microstructural statistics can be correlated to the final product performance. However, this method has challenges associated with the chosen microstructure descriptor and material model. To help illustrate some of these challenges and potential solutions, the application of a void mechanics based constitutive law to reconstructed images will be described below.



Additionally, methodologies for computational evaluation of fatigue properties will be discussed.

## 5.1 Experimental Image Reconstruction Techniques

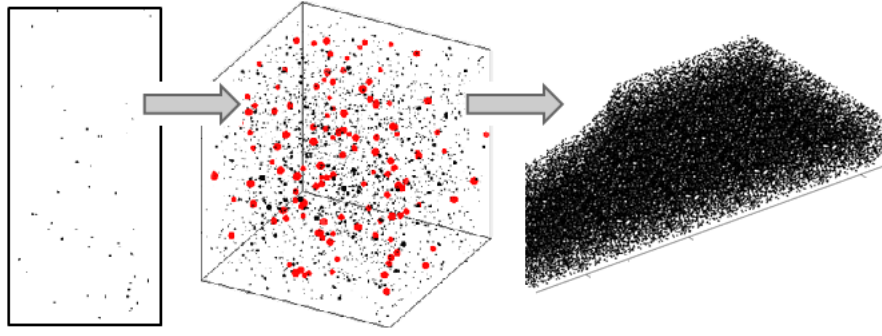
In order to obtain the realistic 3D void distribution in as-built alloys, which can be used as the input for FEM mechanical behavior simulations, optical metallography (OM), SEM (Scanning Electron Microscopy) and FIB (Focused Ion Beam) are adopted as the microstructural characterization tools. OM imaging can provide a good understanding of the overall distribution of distinctly large pores, which are often caused by insufficient fusion. Dual-Beam systems FIB-SEM (FEI Strata DB 235 microscope) are used to conduct multiple 2D serial sectioning to obtain 2D layer images which are then assembled to form a 3D volume representation of the defects using the Amira™ software. Technical details regarding 3D FIB-SEM reconstruction can be found in the work performed by O’Keeffe [12]. It should be noted that FIB-SEM is capable of determining the submicron size of the voids/inclusions, while OM is able to provide an overall distribution of defects in a larger scale. Therefore, a combined technique of OM and FIB-SEM should be applied to gain deeper insight into the size distribution of voids in all length scales. Since FIB-SEM 3D tomography is usually extremely time consuming compared to 2D imaging, 2D OM/SEM microstructural imaging at different locations is considered as an alternative to perform a rapid analysis by sacrificing the precision in 3D volume information. This could be applied as a compromise when performing model testing in preparation for a more rigorous mechanical simulation. Figure 8 illustrates the FIB-SEM 3D reconstructed pore and voids distribution in the LENS processed SS316L sample made for Charpy notch test.



**Figure 8.** Illustration of the 3D tomography using FIB-SEM dual systems. Z is the building direction for LENS processed 316L stainless steel. White dots are reconstructed pores and voids in the Charpy Notch bar made by AM 316L stainless steel sample.

## 5.2 Image-based Mechanistic Plasticity for AM Material

In the ductile fracture process, large deformation cause voids to nucleate, grow, and coalesce which will ultimately cause fracture of the material; the nucleation of new voids is generally initiated at inclusion sites. This can be accounted for in computational analysis of the material through the use of the proper constitutive relations. Assuming that the constitutive relation incorporates the microstructural descriptors of interest, e.g., voids and inclusions, the contribution of these descriptors can be accounted for in the overall material response. The 3D reconstructed volume shown in Figure 8, which includes spatial and volumetric descriptors for defects, can be placed into a simulated component by correlating each defect with the element that encompasses it in physical space, as seen in Figure 9.



**Figure 9.** 3D void and inclusion volume statistically reconstructed from 2D OM/SEM images and microstructure placement into a tensile coupon mesh for experimental validation.

The selection of a material model can be a major challenge. In the case of these SS316L specimens, microvoids can be up to six orders of magnitude smaller than the tensile coupon being simulated. Explicitly modeling each defect using DNS approaches is computationally infeasible. Therefore, one potential method of overcoming this limitation is to use an implicit defect-modeling constitutive law. The Gurson-Tvergaard-Needleman (GTN) is a plastic damage model suitable for this purpose [13]. The yield criterion (Equation 2), which is a function of the local void volume fraction  $f$ , and evolution equations for growth of the local void volume fraction (Equation 3) due to volumetric plastic strain (Equation 4), void nucleation (Equation 5), and shear loading (Equation 6) are [13, 14, 15],

$$\bar{\phi} = \left(\frac{\sigma_{eq}}{\bar{\sigma}}\right)^2 + 2f\beta_1 \cosh\left(\frac{\beta_2 \sigma : \mathbf{I}}{2\bar{\sigma}}\right) - (\beta_1 f)^2 - 1 = 0 \quad (2)$$

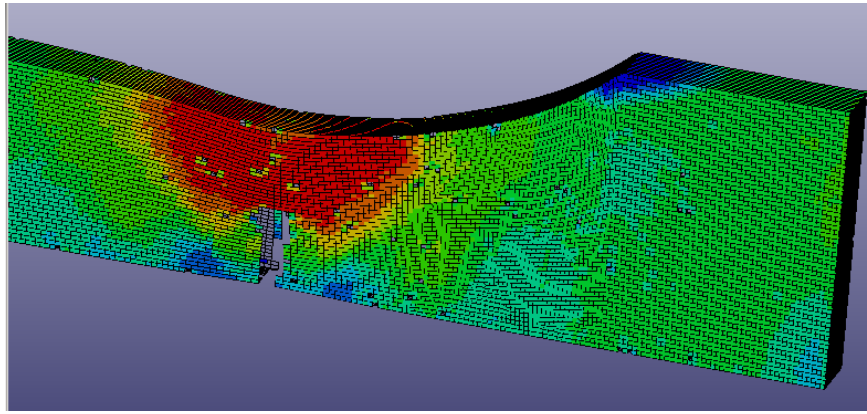
$$\dot{f} = \dot{f}_{growth} + \dot{f}_{nucl} + \dot{f}_{shear} \quad (3)$$

$$\dot{f}_{growth} = (1-f) \text{tr}(\dot{\epsilon}^p) \quad (4)$$

$$\dot{f}_{nucl} = \mathcal{A} \dot{\epsilon}^p + \mathcal{B} \left(\dot{\bar{\sigma}} + \frac{1}{3} \dot{\sigma} : \mathbf{I}\right) \quad (5)$$

$$\dot{f}_{shear} = k_\omega f \omega(\sigma) \frac{(1-f)\bar{\sigma}}{\sigma_{eq}} \dot{\epsilon}^p \quad (6)$$

The higher the defect volume fraction, the weaker the element. The GTN model has demonstrated potential for capturing material across widely varying length scales. Previous work from Tang [16] and O’Keeffe [12] showed that image-based techniques combined with the GTN model could be used to effectively simulate crack openings by explicitly accounting for primary micron scale defects and using multiresolution theory for submicron scale defects. For the simulation of macroscale components, the GTN model should be implemented for much larger microstructural features with an emphasis on computational efficiency. Figure 10 shows a finite element simulation of a void-embedded tensile coupon. This combination allows what would normally be considered calibration parameters related to the microstructural defects within the GTN model, i.e., void and inclusion distributions, to simply be experimentally derived inputs. The residual GTN model parameters can be decoupled and calibrated using experimental tests specific to the sensitivity of each parameter. For example, the hydrostatic growth term can be decoupled from shear effects [15, 17] and varied parametrically; temperature and strain rate effects can also be isolated.



**Figure 10.** Void driven fracture of a tensile specimen embedded with image-based microstructure information in a finite element simulation with the GTN constitutive model

The role of the microstructure and the structure-property relationship on the overall performance of AM materials cannot be ignored. The GTN model as a case-study has demonstrated the potential for experimentally-informed microstructural descriptors to be integrated into advanced material modeling techniques which incorporate microstructural conformation and constituent characteristics. Advanced image-based techniques are a promising direction for exploring the link between structure and performance in metal-based AM.

### 5.3 Multiscale Fatigue Modeling for AM

Mechanistic modeling of monotonic loading and the resulting mechanical response is a valuable endeavor; however, in most structural applications, component design must account for fluctuating loads and the progression of failure due to such loads, i.e., fatigue. To advance metal-based AM to the next level, mechanical fatigue modeling and accurate fatigue life prediction for functional AM components is necessary. Generally poor to fair fatigue performance of AM material is often acknowledged by authors studying the topic; it is most often attributed to (1) defects such as voids (micro-pores) and microcracks, (2) high residual stresses, (3) poor as-built surface finish, and (4) microstructural conformation [18,19,20,21,22]. However, the importance of each of these factors varies depending upon the specifics of the study, including: manufacturing process (SLM is commonly used for fatigue studies), material (titanium/steel alloys and nickel-based superalloys are common), and loading condition (low versus high cycle fatigue).

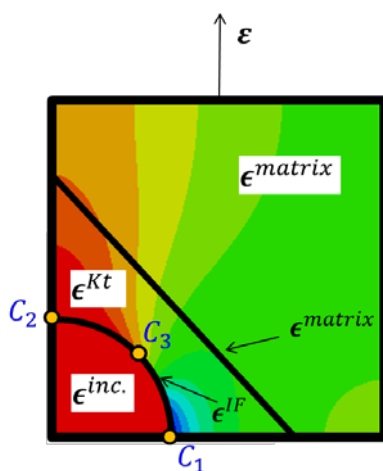
While several groups have considered fatigue loading for AM parts experimentally, to our knowledge a mechanistic model of fatigue in AM materials has yet to be proposed. Efforts to adapt conventional fatigue models to AM processed materials, most notably that of Leuders and coworkers [23], have yielded limited success. While some conditions are captured well by adaptations of existing phenomenological models for Ti-6Al-4V processed with SLM, e.g., the  $\sqrt{\text{area}}$  model and the Danninger-Weiss model (see [23] for details), such models yet fail to accurately capture fatigue life of post-processed and as-built materials, respectively [23]. Wycisk *et al.* [24] take a slightly different approach, modeling fatigue crack growth using linear elastic fracture mechanics to determine crack propagation and final failure with the El Haddad and Topper approach. Use of classical fatigue stress-life methods such as the Paterson and Neuber equations are contraindicated by Lipinski *et al.* [25], at least for the case of thin-walled structures, though a proposed notch stress-gradient approach was more successful in predicting fatigue strength in medical grade 2 Titanium. In this approach, the stress gradient at the expected crack location is determined from monotonic loading and used to define a fatigue concentration factor through fitting experimental results; the resultant apparent stress was used to assess failure of the structure. This approach appears to work satisfactorily to account for notches in parts with controlled porosity, though fails to account for particular microstructures that may interact to deleterious effect.

Here, we shall focus on development of a multiscale mechanistic model of fatigue tailored to AM. A multiscale model is required due to the disparity of scales involved. Fatigue life depends upon interactions between microstructural defects and macrostructural geometric features. Further specifying AM for the present study, and even powder bed or direct deposition processes specifically, constrains our modeling effort to the four primary fatigue-influencing parameters defined above. We propose to employ the multiscale fatigue model developed by Moore [26]. This model is based on two classic micromechanics laws,

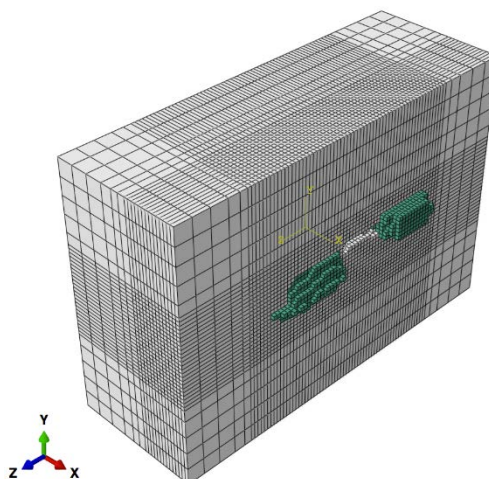
$$\boldsymbol{\varepsilon} = \frac{1}{\Omega} \int_{\Omega} \boldsymbol{\varepsilon}(\mathbf{x}') d\Omega \quad (7)$$

$$\llbracket \mathbf{n} \cdot \boldsymbol{\sigma} \rrbracket = 0 \quad (8)$$

The first equality, shown in Equation (7), is used to relate macroscale strain,  $\boldsymbol{\varepsilon}$ , to micro-strain,  $\boldsymbol{\varepsilon}$ , which is a function of the microscale coordinate over the micro-domain  $\Omega$ . The second equality, shown in Equation (8), is used to enforce continuity of force across weak interfaces, where  $\mathbf{n}$  is the interface normal and  $\boldsymbol{\sigma}$  is the microscale Cauchy stress. Moore then enforces these conditions only at key points as shown in Figure 11, allowing for a fast and flexible model.



**Figure 11.** Strain continuity assumptions for microscale constitutive law, overlaid over stress profile from highly detailed FEM calculations. Continuity points for xx-, yy-, and xy-stress components are  $C_1$ ,  $C_2$ , and  $C_3$  respectively [26].



**Figure 12.** Reconstructed mesh from image data with two oxide inclusions, slide to highlight the oxides and interstitial void. This was used to calibrate the model.

To apply this to AM, a computational plasticity model is developed to capture defects, residual stresses, and local microstructure. The approach that we propose is based on the 3D image-based analysis similar to that of Moore (see Figure 12 for an example of a meshed

image used by Moore), which has been developed in conjunction with a multiscale fatigue model that focuses on the effects of voids, inclusions, and their interactions on fatigue life [26]. Moore’s work uses models informed by detailed crystal plasticity calculations calibrated with a statistical volume element. While intractable to use directly in a multiscale model, this can provide key insights into the nature of fatigue failures and can be used to inform development of simpler constitutive laws.

In the case of AM, a similar approach using a dataset trained from 3D reconstructions of AM microstructures (see Figure 8) will be used to inform constitutive law development to be applied to Moore’s multiscale fatigue model. The new constitutive law must compute strain gradients to allow adaption of the microstructure to changes in geometry, material, and additional nonlinearities. This constitutive law will then be used to compute local microstructural plasticity coupled to the FEM at the macroscale to compute component response. The physically based microscale information required to assess fatigue life will be retained, as Moore describes [26].

## 6 METHODS FOR IMAGE-BASED CONSTITUTIVE LAW DEVELOPMENT

The complexity in the material properties and the hierarchical anisotropic microstructure of additively manufactured materials necessitates development of new advanced material models. In most practical applications, e.g., metal forming, new material models are developed for specific materials under the specific loading conditions of the process using both phenomenological and mechanically-based techniques but typically these material models are neither versatile nor extensible. The versatility of the process parameters in AM combined with the resulting process-structure-property relations tend to leave traditional material modeling techniques useless. An ideal solution is then to develop a framework which can be used to quickly create new material models based on either structure, property, or a combination of the two.

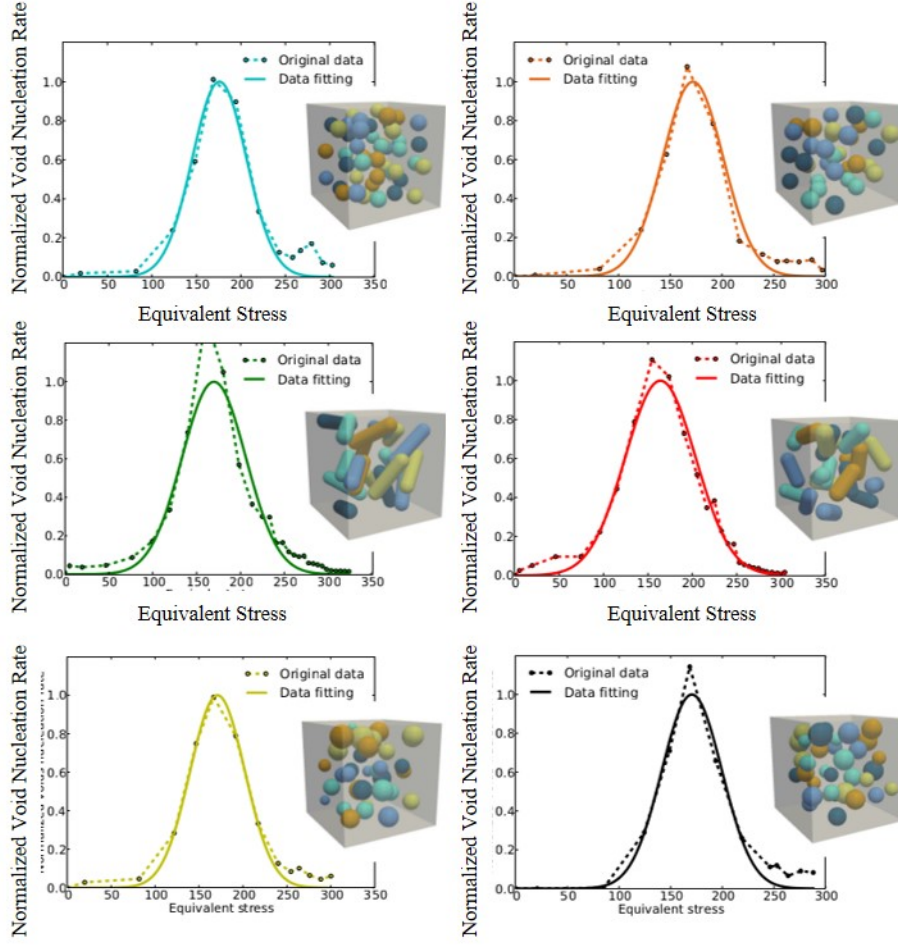
The eXtended Finite Element Method (XFEM) incorporates an enrichment of the standard finite element shape function such that strong and weak discontinuities can be captured without the need for a conforming mesh. While this method is typically used for interfaces, crack initiation, propagation, and fracture, it can just as easily be applied to represent a multi-phase microstructure. This has a lot of potential when microstructure descriptors from modern imaging techniques are so readily available. While it would be computationally prohibitive to perform analysis over a large domain using XFEM, it is still possible to rapidly generate statistically representative domains which can be used for development of homogenized material model development. This is a tremendous advantage compared to standard finite element analysis which is extremely costly in terms of meshing time. The impact of the material microstructure, and therefore the structure-property relation, can then be taken into account when developing the new model either explicitly or implicitly based on the microstructure descriptors. The stochastic properties can also be conserved using the methodology which is great for uncertainty quantification.

An example of this methodology can be observed in Figure 13. The six different material domains are composed of a large distribution of inclusions with varying microstructural conformations, i.e., elongated ellipsoidal and spherical constituents with random distributions. These domains were meshed using XFEM and the void nucleation rate was recorded for triaxial loading conditions. Void nucleation was dictated by a cohesive law at the matrix-constituent interface. From the results, a physically relevant void nucleation theory for this material can be developed based on the microstructure descriptors available for the material, e.g., inclusion distribution and directional properties. One such XFEM-derived nucleation law which holds for hydrostatic, shear, and triaxial load conditions for spherical inclusions can be written as [27],

$$B(\sigma_{eq}) = \frac{f_N}{\sigma_y \sigma_s \sqrt{2\pi}} \exp\left(-\frac{1}{2} \left[ \frac{\sigma_{eq} - \sigma_N}{\sigma_y \sigma_s} \right]^2\right) \quad (9)$$



where  $f_N$  is the volume fraction of the nucleatable void,  $\sigma_N$  is the mean nucleation stress,  $\sigma_s$  is the standard deviation of the mean nucleation stress,  $\sigma_y$  is the initial yield stress, and  $\sigma_{eq}$  is the equivalent stress. This is similar, but not equivalent, to that proposed by Tvergaard and Needleman [14] for usage within the evolutionary equation for voids in the well-known Gurson model [13].



**Figure 13.** Void nucleation rate as a function of equivalent stress for various microstructure conformations [27].

Another possibility for predicting AM material properties through material modeling is through the use of generalized material modeling frameworks. Instead of developing material-specific models, this technique would simply make an assumption of the types of mechanics which may be necessary for a given material class and, through generalized stress invariant functions, novel material models can be developed using a methodical procedure. For example,

$$\phi^* = \bar{\phi}^\xi + \eta(I_1^*) - \beta(I_1^*)\bar{\sigma}^\psi \leq 0 \quad (10)$$

where  $\phi^*$  represents the yielding condition for plasticity,  $\bar{\phi}$  represents an effective stress value in the reference frame of interest [28],  $\eta(I_1^*)$  represents a generalized additive pressure dependence function,  $\beta(I_1^*)$  represents a generalized multiplicative pressure dependence function,  $\bar{\sigma}$  represents the matrix flow stress,  $\xi$  represents the nonlinearity of the yield surface, and  $\psi$  represents a parameter for ensuring consistent units within the yield condition. This approach is convenient for computational material modeling because the resulting implementation need only be successfully developed once and then it can simply be used as a template for new models. New model implementation would then require definition of the governing equations. The nature of the material modeling framework also implies that incorporating microstructure effects either through phenomenological approaches or using mechanics-based theories is still an option. Extension of existing material models is also

simplified, e.g., extension of an isotropic pressure-dependent model to anisotropy. This methodology could be used to incorporate image-based microstructural effects by combining the function

$$\beta(I_1^*) = \sqrt{1 + (q_1 f^*)^2 - 2f^* q_1 \cosh\left(\frac{q_2 I_1^*}{2\bar{\sigma}}\right)} \quad (11)$$

with equations (9) and (10) such that void-induced weakening is obtained ( $q_1$  and  $q_2$  are yield function shaping parameters and  $f^*$  is an effective void volume fraction) but the form of the effective stress used and the hardening imposed through the matrix flow stress equation can still be altered based on other microstructural/mechanistic or phenomenological influences.

## 7 CONCLUSIONS

AM of metallic materials is a rapidly flourishing field fostering synergistic interactions among disciplines for challenges and opportunities. For example, AM products are characterized by high porosity and anisotropic material behavior and microstructures which introduce difficulty in predicting the final product behavior, thus delaying the presence of AM in the industrial sector. These phenomena are not unique to any particular material or material class, e.g. titanium alloys and stainless steels both have these traits. The process parameters clearly have a profound effect on the overall performance of AM products. This necessitates the development of efficient methodologies for assessing AM products and developing computational tools to assist in the prediction of process-structure-property relations.

The strength of using experimentally-informed mechanistic models lies in the efficient use and analysis of the structure and performance data obtained in a single experiment; this is a practical way of determining how well their relationship can be explained by developed material models. By choosing a constitutive law that can incorporate image-based microstructure, the parameters to be calibrated are reduced and the accuracy of mechanical predictions for simulated components can be improved. A well-chosen material descriptor, when combined with a general constitutive law, provides a flexible material model that can accommodate a variety of microstructural distributions. The implementation of the GTN model on OM/FIB-SEM reconstructions of void and inclusion data holds promising quantitative results for the multiscale simulation of ductile deformation and fracture, ranging from defects of submicron scale to parts on the macroscale. The reduced order microstructural modeling based on advanced data compression provides an efficient and accurate tool for the image-based constitutive modeling.

While some experimental efforts to characterize the fatigue response of AM processed parts has been published, very little has been published on fatigue simulation and life prediction. Only three papers thus far attempt to predict fatigue life specifically for AM to our knowledge, all of which rely on macroscale fitting of experimental results, limiting the broader applicability and mechanistic completeness of the studies. Here, we propose a mechanics based multiscale method to predict fatigue life with microscale constituencies informed by AM-specific parameter. The proposed model predicts macroscale fatigue response while maintaining the necessary microscale information. Development of a multiscale fatigue model tailored to AM allows for more informed topological design of components through the addition of a fatigue resistance criterion. Furthermore, the importance of microstructural defects and their location can be assessed to help inform AM process and process design choices.

The need for novel techniques which allow development of image-based constitutive modeling techniques has been discussed. Two proposed methods for realizing a solution for this need have been presented: (1) an XFEM-based methodology which can be used to quickly reconstruct image-derived microstructures within stochastic properties and (2) the concept of a constitutive model development framework which uses generalized stress invariant functions which can be tailored for each material and can incorporate microstructural effects. The purpose of these methods is to allow for a simple and efficient procedure for constitutive model development. The implications that these methods have for AM are many. The primary benefit

is in the fact that AM product material behavior is unique in that powder composition does not necessarily govern the overall response, i.e., microstructural descriptors are of equal (if not more) importance.

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