Direct numerical simulation of mechanical response in synthetic additively manufactured microstructures

Theron M Rodgers\textsuperscript{1,4}, Joseph E Bishop\textsuperscript{2} and Jonathan D Madison\textsuperscript{3}

\textsuperscript{1} Computational Materials & Data Science, Sandia National Laboratories, PO Box 5800 MS-1411, Albuquerque, NM 87185, United States of America
\textsuperscript{2} Solid Mechanics, Sandia National Laboratories, PO Box 5800 MS-0840, Albuquerque, NM 87185, United States of America
\textsuperscript{3} Materials Mechanics, Sandia National Laboratories, PO Box 5800 MS-0889, Albuquerque, NM 87185, United States of America

E-mail: trodger@sandia.gov, jebisho@sandia.gov and jdmadis@sandia.gov

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Abstract
Additive manufacturing (AM) processes for metals can yield as-built microstructures that vary significantly from their cast or wrought counterparts. These microstructural variations can in turn, have profound effects on the properties of a component. Here, a modeling methodology is presented to investigate microstructurally-influenced mechanical response in additively manufactured structures via direct numerical simulation. Three-dimensional, synthetic voxelized microstructures are generated by kinetic Monte Carlo (kMC) additive manufacturing process simulations performed at four scan speeds to create a thin-wall cylindrical geometry notionally constructed using a concentric-pathed directed energy deposition AM process. The kMC simulations utilize a steady-state molten pool geometry that is held constant throughout the study. Resultant microstructures are mapped onto a highly-refined conformal finite-element mesh of a part geometry. A grain-scale anisotropic crystal elasticity model is then used to represent the constitutive response of each grain. The response of the structure subjected to relatively simple load conditions is studied in order to provide understanding of both the influence of AM
processing on microstructure as well as the microstructure’s influence on the macroscale mechanical response.

Keywords: additive manufacturing, Potts Monte Carlo, SPPARKS, direct numerical simulation

(Some figures may appear in colour only in the online journal)

1. Introduction

1.1. Review of simulation techniques for metal additive manufacturing microstructure formation

Many promising applications for metal additive manufacturing (AM) involve replacing traditional cast or wrought components with tailored as-built geometries wherein shape complexity is no longer a limiting factor [1, 2]. Unfortunately, the complicated thermal histories present in AM builds can result in abnormal microstructural morphologies and/or properties [3, 4]. Additionally, to leverage the full benefit of AM and near-net shape builds, one would prefer to generate as-built parts with minimal to no post-processing. Furthermore, even in instances of hot isostatic pressing and/or subsequent heat treatment, the initial microstructure will always influence the post-processed result. Thus, an understanding of as-built AM microstructures and their impact on performance is currently a subject of high value and interest.

The prediction of as-built AM microstructures is a rapidly expanding field of study. A variety of prediction methods have been developed for analysis at the macroscopic length scale. Examples include the creation of laser-based process-parameter maps [5, 6] and the use of classical finite-element (FE) simulations to assess thermal histories with empirical models for microstructure-property prediction [7]. These predictions are largely focused on bulk or homogenized properties and in their current form, provide little in the way of microstructural prediction at the melt pool scale. At smaller length scales, there is significant interest in the effects of process conditions (most notably undercooling) on dendritic solidification. These models can incorporate alloy effects such as solute segregation and the dendritic/cellular/planar transitions [8–10]. These simulations typically employ phase field or micro-cellular automata (CA) techniques and are currently too computationally expensive to simulate more than a handful of three-dimensional dendrites.

In contrast to these methods, more straight-forward simulations of meso-scale grain evolution are also under development. Many of these approaches utilize adaptations of the cellular automata-FE approach initially developed in the 1990s to simulate grain formation during casting [11, 12]. This method has been extended to model grain formation during welding and cladding [13], and a few AM solidification approaches have also adopted the CA solidification scheme as well [14–16]. DebRoy et al have developed a more empirical approach to predict solidified grain shapes by incorporating a rigorous description of fluid flow and heat transfer in the molten zone with a Monte Carlo (MC) model of grain evolution [17–19]. Alternatively, by using solidification front velocity and thermal gradient estimations as an initial approximation for solidification conditions, Rodgers et al have developed a modified Potts Monte Carlo approach for prediction of solidified grain structure following welding or additive manufacturing [20, 21]. Unlike other methods, this MC-based approach allows for the generation of three-dimensional microstructures consisting of hundreds of build layers each with multiple laser passes. Due to the computational efficiency and scalability of the approach, it offers unique opportunities to directly simulate significantly sized domains,
and evaluate simulation results with data mining techniques to assess relationships between simulated process histories and grain structure \cite{22}. Additionally, these large domains also make utilization of their outputs both suitable and attractive for comparison and integration with additional simulation efforts as will be discussed next.

The incorporation of microstructure within mechanics simulation is also a burgeoning field. At present, microstructural surrogates such as Voronoi tessellations are commonly used \cite{23, 24}. Aside from the documented shortcoming of such microstructural substitutes \cite{25}, one less appreciated challenge is the mapping of microstructures generated on a voxelized grid (e.g. cellular automata and Potts Monte Carlo) or those having diffuse boundaries (e.g. phase field) onto FE meshes. Further constraints are also imposed by the number of elements FE methods can tractably include within a single grain; thereby limiting the fidelity of grain boundaries and resolution within grain interiors. There is ongoing work to enable conformal meshing of grains \cite{26, 27}, but these methods are not yet adept at modeling large-scale three-dimensional microstructures.

The simulations performed here represent an attempt to reasonably address many of the aforementioned shortcomings in AM simulation by connecting several of the linkages in the idealized process-structure-property-performance framework shown in figure 1. Currently, the simulation and analysis methods at each node are typically well established. However, the linkages between the nodes are often ill-defined and application-dependent. For engineering applications, additional consideration must be given to length- and time-scale considerations, as many properties (and computational approaches) are most active at specific scales and either impractical or intractable when applied to another length scale or time domain.

Here, Monte Carlo generated microstructures are used in direct numerical simulations (DNS) of mechanical behavior in the elastic regime. Multiple, three-dimensional microstructure instantiations for a tubular AM build are generated at four different laser scan speeds, which result in microstructures with differing grain size distributions and grain morphologies. The voxelized MC microstructures are then mapped to a FE mesh and grain orientations are specified from a uniform random distribution. Simple loading conditions of tension and torsion are applied to provide insight into the effects of grain-scale heterogeneity on the mechanical response. A more complex stress state was also examined by virtually ‘milling’ a side hole through the tube walls. Ultimately, the microstructure-dependent von Mises stress response is analyzed in Fourier space to provide a quantitative description of

Figure 1. Schematic illustrating the fundamental process–structure–property–performance relationship for materials with a focus on simulation tools applicable to additive manufacturing.
strain heterogeneity influenced by local and long-range microstructural arrangements across all cases. Section 2 will provide an overview of the kinetic Monte Carlo (kMC) and DNS simulation methods while section 3 will present the results of each method for several processing conditions and mechanical loading states. Sections 4 and 5 will provide discussion and conclusions to summarize the work.

2. Simulation methods

This section will discuss the simulation techniques used in this study. Sections 2.1 and 2.2 will focus on the Potts Monte Carlo-based technique used to generate synthetic microstructures. Sections 2.3 and 2.4 will present the definition of the FE mesh used in the mechanics simulations as well as the mapping between the kMC and FE meshes. Sections 2.5 and 2.6 shall discuss the details of the mechanical constitutive model and the DNS simulations.

2.1. Additive manufacturing microstructure model

Microstructures were generated using a modified Potts kMC model previously described in [20]. Here, only the essentials of the model, along with modifications for cylindrical domains will be discussed. The reader is directed to the aforementioned reference for additional details. The model is based on the Potts model for curvature driven grain growth [28] in which grains are defined by assigning a unique integer ID to each grain. Contiguous lattice sites possessing the same ID value are considered a grain. Grain evolution occurs by performing ID-flips at neighboring sites having unlike IDs following Metropolis dynamics:

\[ P = \begin{cases} \frac{-\Delta E}{k_B T} e^{\Delta E/k_B T}, & \text{if } \Delta E > 0 \\ 1, & \text{if } \Delta E \leq 0, \end{cases} \]  

where \( k_B \) is the Boltzmann constant, \( T \) is the Metropolis simulation temperature and \( \Delta E \) is the change in system energy cause by the exchange. Here, \( T = 0 \), which prevents flips that would increase the system energy [29]. With this change, equation (1) reduces to:

\[ P = \begin{cases} 0, & \text{if } \Delta E > 0 \\ 1, & \text{if } \Delta E \leq 0. \end{cases} \]  

To model solidification phenomena, three primary modifications to the Potts model are introduced; a molten zone, a surrounding heat-affected zone (HAZ) and a temperature dependent grain boundary mobility. The ‘molten zone’ corresponds to a region of space in which temperature exceeds the melting point of the material. In this region IDs are randomized every timestep (mimicking the disorder present in a molten system). Upon exiting the molten zone, sites enter a high thermal gradient, HAZ and grain evolution can occur following Metropolis dynamics (as in the standard Potts model), but with a temperature dependent mobility prefactor. This mobility takes the following form:

\[ M(T) = M_0 e^{-Q/RT}, \]  

where \( M_0 \) is a user-defined prefactor, \( Q \) is the activation energy for grain boundary motion (assumed constant), \( R \) is the gas constant, and \( T \) corresponds to the temperature gradient surrounding the molten zone. The determination of these parameters is described in [20]. The mobility prefactor modifies equation (2) as follows:
While the molten zone’s position is constantly moving within the simulation domain, the molten zone and surrounding HAZ is approximated by a steady-state, user-defined geometric parameter set (including length, width, and depth) described in [20]. The previous reference utilized rectilinear scan patterns, while here a circular pattern is used, as shown in figure 2. Thus, the molten zone shape parameters are translated into cylindrical coordinates, and the molten and HAZ lengths are specified as a circular arc length. This configuration allows the specification of a curved molten zone that follows the arc of the scan pattern.

2.2. Study-specific kMC parameters

A hollow tube geometry having an outer diameter ten times and a length 30 times its wall thickness (figure 2) was selected for the study. The geometry is straightforward to implement in the present model but offers an increase in complexity from rectilinear or closed body domains commonly used in many AM simulations [19, 30, 31]. A two-pass concentric-circular scan pattern was implemented, analogous to patterns used in directed energy deposition (DED) and other powder-fed AM techniques [32, 33]. For all builds in this study, two concentric passes were used on each layer as shown in figure 2(a). Powder-bed methods typically utilize smaller laser spot sizes with correspondingly smaller molten zones. For the exemplar shown here, it is reasonable to expect powder bed approaches to require more complex scan strategies (corresponding to longer simulations times) to successfully build a tube of this dimension. For the sake of efficiency, the AM microstructure generation model simulated an AM process with 100 build layers and two scan passes per layer in accordance with capability recently demonstrated using DED approaches [34].

No physical length scale is explicitly included in the Monte Carlo simulations, but a scale is implied through the dimensions of the cylindrical domain, melt pool size, and scan pattern. In order to reflect the dimensions of a typical experimental DED process, a voxel size of 25 μm was determined for the simulation length scale [35]. This results in a molten zone width of 0.5 mm, a layer height of 0.3 mm, and a cylinder height of 30 mm.

Similarly, physical time is also not explicit in Monte Carlo simulations. Instead, time evolution is typically expressed in units of Monte Carlo steps (MCS). An MCS is defined as performing one Monte Carlo test at all lattice sites within the simulation domain. Lattice sites that have zero probability to change (due to not having any unlike neighbors or having a mobility of zero) can be skipped without changing the MCS interval. It can be assumed that

\[
P = \begin{cases}
0, & \text{if } \Delta E > 0 \\
M(T), & \text{if } \Delta E \leq 0.
\end{cases}
\]
the relationship between MCS and real time is linear. However, the exact relationship is dependent on the model implementation and material system studied [20, 36, 37]. This relationship for Monte Carlo simulations of solidification is yet-to-be explored and will be studied in future work. However, a relationship can be approximated from experimental microstructures. A scaling factor of 0.0012 s/MCS was found to correspond well to experimentally observed microstructures within the simulated region.

A variety of as-built synthetic microstructures were created in accordance with the geometry described above by varying the molten pool’s scan speed. The scan speed was varied across four specific speeds; 4, 8, 10, and 16 mm s\(^{-1}\) as these produced the full spectrum of columnar to equiaxed grain morphologies. This trend in microstructure variation is also reflected in experimental results with columnar grains present within the low range [34] and mixed columnar/equiaxed microstructures found at higher speeds [33, 35]. All other simulation parameters were held constant (including the molten pool geometry and HAZ dimensions), and are summarized in table 1. Several of these parameters (pool width, length, depth, HAZ width, and cap height) define the shape of the molten zone and heat-affected regions, while the others (minimum radius and hatch spacing) define the scan pattern used.

The molten pool geometry is defined as a pair of ellipsoids that meet at their midplane (perpendicular to the scan direction) and share two axes (pool width and depth). The third axis of the molten pool (pool length and cap length) is parallel to the scan direction. Ellipsoids are defined using the cylindrical coordinates of the part shape, such that the length axes follow the cylinder circumference, width axes are parallel to the radius and depth axes are parallel to Z (the build direction) as shown in figure 2(a). HAZ width is the maximum width of the ellipsoids that define the heat-affected region surrounding the molten pool. It is defined as parallel to pool width and extends beyond the molten pool. The resulting HAZ is shown in blue in figure 2(a). Outside of the HAZ ellipsoid, the temperature is low enough that no significant microstructural evolution occurs. Lastly, for the scan pattern, minimum radius defines the midline of the inner-most scan circle, and hatch spacing is the distance between the two rastering melt pool centers.

### 2.3. Definition of tube domain with kMC and FEA discretization

A schematic of the tube used in simulation is shown in figure 2 with dimensions indicated in mm. The domain is shown after a side-hole was virtually ‘machined’ out of the tube wall at the midpoint along its length. The results of the geometry with a side hole will be discussed in section 3. The coarse conformal FE mesh of the tube including the side-hole is shown in figure 3. This base FE mesh was hierarchically refined multiple times in which each hexahedral element was subdivided into eight new elements. The finest meshes consisted of 22,151,168 and 29,622,272 elements for the tube and tube with side-hole, respectively. An example of the refined mesh is shown on the right side of figure 3. Although neither the kMC nor the crystal elasticity simulations contain an inherent length scale, the simulation’s relationship with experimental conditions is imposed by the ratio of the tube’s wall thickness to the number of grains through the wall thickness.

| Simulation parameter | Pool width (mm) | Pool length (mm) | Pool depth (mm) | HAZ width (mm) | Cap length (mm) | Minimum radius (mm) | Hatch spacing (mm) |
|----------------------|----------------|-----------------|----------------|---------------|-----------------|---------------------|-------------------|
| Value                | 0.5            | 0.625           | 0.45           | 0.875         | 0.25            | 4.25                | 0.5               |
2.4. Mapping voxelized kMC microstructures to conformal FEs

The meshing of polycrystalline grains that reliably conform to grain boundaries is extremely challenging and typically requires user intervention. This need for user intervention increases with the number of grains and the complexity of the geometry. Furthermore, constructing a volumetric FE mesh that is conformal with both the geometry and the microstructure is even more challenging. As a result, this meshing challenge is currently an active area of research [26, 36–39]. A computational methodology for directly embedding polycrystalline microstructures within a macroscale structure has been recently proposed and explored by Bishop et al [23, 24]. While alternative methods for microstructural realization have been used by others [40–42], Bishop’s approach, a type of DNS, is adopted here and is briefly reviewed in the following sections.

In this work, grain morphologies are defined through the kMC simulations and are thus inherently voxelated. For this reason, in the structural analyses an approach is adopted in which the macroscale structure (a tube with or without a side hole) is meshed conformally with hexahedral elements, and the grain membership of each hexahedral element is determined by the value of the nearest kMC voxel in the original microstructure. This is a common technique in the modeling of composite and polycrystalline microstructures within a representative volume element (RVE) [43, 44].

The resulting conformal FE meshes of the tube had 32 elements through the thickness of the tube, while the original kMC voxelation had roughly 40 voxels through the tube thickness. Thus, the mapping of the kMC grain structure to the FE mesh of the tube required a 20% down sampling in resolution. An example of the resulting mapped microstructure (along with the original kMC grid) is shown in figure 4. Comparison of the original and meshed microstructures show that little detail was lost in the mapping, and the kMC grains retain their characteristic shapes and sizes. The mapped microstructure is conformal to the tube geometry, but still voxelated at the grain boundaries.

2.5. Mechanical constitutive model and crystal orientations

The material model used in this study was AISI 304 L stainless steel. This material possesses an austenitic γ-Fe microstructure within an FCC crystal system. In the plastic regime, the mechanical response of each FCC grain can be modeled using an elasto-viscoplastic crystal plasticity as described by Bishop [23]. As mentioned previously, in this work, only the elastic
regime is explored to document and present the approach. For the elastic response, the austenite FCC crystal structure possesses cubic symmetry with elastic constants $C_{11} = 204.6$ GPa, $C_{12} = 137.7$ GPa, and $C_{44} = 126.2$ GPa [45]. The anisotropy ratio, $A$, for this crystal is $A = 2 \frac{C_{44}}{(C_{11} - C_{12})} = 3.77$, which is relatively large. For an isotropic material, $A = 1$.

Each voxel within a grain is given the same crystal orientation. While very general crystal textures could be modeled, to avoid unnecessary convolution of the results, the distribution of grain orientations is taken to be uniformly random (i.e. no preferred texture). There is also no spatial correlation in the grain orientations. Care is needed in randomly assigning the grain orientations to realize a no-texture state (see, for example, [46, 47]). In the absence of a crystal texture, the homogenized mechanical response of the material is isotropic. The effective (homogenized) elastic mechanical properties have been obtained by Bishop [24] using an idealized equiaxed Voronoi microstructure. The effective Young’s modulus and Poisson’s ratio are 197.6 GPa and 0.294, respectively.

2.6. DNS simulations

To simulate the tube structures using the highly-refined FE meshes shown in figures 3 and 4, a massively parallel solid mechanics code that can scale efficiently to thousands of processors is required. In this work, we use the quasi-static solid mechanics module within the Sierra multiphysics FE software suite [48]. The FETI-DP equation solver was used for all simulations. FETI-DP is a domain-decomposition iterative solver that uses Lagrangian multipliers to enforce compatibility at the subdomain interfaces [49].

Typical simulations used over 1000 processors but required less than an hour of clock time since only loading in the elastic regime was considered. Future work will consider
loading into the plastic regime as described in [23]. Simulations in the plastic regime typically require many days of clock time.

3. Results

This section presents the results of the microstructure generation model and DNS simulations. Section 3.1 discusses the kMC microstructures generated at four processing conditions. Section 3.2 then presents the results of mechanics simulations incorporating these microstructures for several loading conditions: a solid tube in tension (section 3.2.1), a tube with a side hole in tension (section 3.2.2), and a tube with a side hole in torsion (section 3.2.3). Section 3.3 then analyzes the variation of the mechanical response using discrete Fourier transform (DFT) analysis across all cases.

3.1. kMC microstructures

The range of scan speeds used in the simulations produce microstructures spanning columnar, columnar-to-equiaxed, and fully equiaxed grain morphologies [50, 51]. In the synthetic microstructures depicted here, this is controlled primarily by variation of the solidification front velocity, $V$, which is informed by the scan speed of the molten zone. At low scan speeds, $V$ is small and grain evolution is comparable with the traveling solidification front resulting in epitaxial, columnar growth. As a result, rather large, helical, columnar grains spanning significant lengths of the tube wall form. As scan speeds increase, grains quickly decrease in average size and elongation. To demonstrate this behavior, mid-wall grain microstructures at four scan speeds (4, 8, 10, and 16 mm $s^{-1}$) are shown in figure 5. The images shown were generated by revealing the mid-surface of each cylinder’s wall thickness. Comparison of these synthetic microstructures with experimental results is on-going and reasonable amounts of both qualitative and quantitative agreement have been found [20]. While grain inclinations relative to build direction can be a challenge for build-scale experiments having complex thermal environments, this approach has been shown to accurately predict the columnar to equiaxed transition regardless [34]. As such, this is the primary morphological trend the authors seek to demonstrate and study here.

The two-pass per layer scan strategy results in a more complex microstructure than is immediately apparent from observation at a singular depth into the wall. Generally, regions that undergo remelting and reheating will be more prone to the development of elongated grains than those that interact with the molten zone and HAZ once. This effect is compounded by the remelting of previous layers, which occur often with larger grains near the wall’s midpoint. These events result in continued epitaxial growth. As a result, the mid-surface of the wall thickness experiences the greatest amount of heat input and thus the largest grain sizes. In contrast, the regions near the wall’s surfaces only experience one heating cycle per layer. For this reason, the mid-surface of each tube is shown in figure 5 to provide indication of each cases’ most elongated, columnar grain structure. This most notable difference between midplane and outer surface microstructures is found at the 8 mm $s^{-1}$ case. Here the midplane microstructure (where the two scan passes overlapped) produced very large, columnar grains, while the outer regions (that only received a single pass per layer had much smaller grain sizes).

Grain sizes for each case as a function of distance from the inner diameter are shown in figure 6. The grains’ radial locations were determined by the position of their centroids in the XY plane. At low scan speeds (figure 6(a), 4 and 8 mm $s^{-1}$), the size distributions show a large peak near the mid-surface with maximum grain volumes of 45 and 33.4 mm$^3$ respectively. At
Figure 5. Microstructures at the mid-surface of the tube’s wall thickness. The microstructures show a gradual transition between columnar and equiaxed microstructures with increasing scan speed.

Figure 6. Scatter plot of grain volumes for scan speeds of (a) 4 and 8 mm s$^{-1}$, and (b) 10 and 16 mm s$^{-1}$. Note the order-of-magnitude difference in grain volume scales between the two plots.
a speed of 4 mm s$^{-1}$, secondary peaks (with the largest grains about 40% the volume of those along the centerline) are also shown approximately 0.125 mm from the inner/outer surfaces. This indicates that this speed was slow enough to induce columnar grain formation regions experience only a single pass of the molten pool and HAZ each layer. At a speed of 8 mm s$^{-1}$, large, columnar grains remain along the midplane, but grains are much smaller near the inner/outer surfaces (as also shown in figure 5). At faster scan speeds (figure 6(b), 10 and 16 mm s$^{-1}$), the maximum grain sizes are much smaller (1.1 and 0.18 mm$^3$), and the overall distributions are more spatially uniform. At 10 mm s$^{-1}$ the largest grains along the centerline are an order-of-magnitude larger than those in other regions, while at 16 mm s$^{-1}$, grain sizes varied by less than 0.2 mm$^3$.

3.2. DNS simulations of the mechanical response

DNS simulations were performed on the tube geometries described above. Solid mechanics simulations were carried out for simple tension in the solid and hole-containing tubes. Tubes with machine-drilled holes were additionally examined in torsion. The traction boundary conditions on the end-surfaces at $z = 0$ and $z = 30$ mm (see figure 2) for each load case are given as:

$$
\begin{align*}
 t_x &= 0 \\
 t_y &= 0 \\
 t_z &= -1.0
\end{align*}
$$

at $z = 0$ and

$$
\begin{align*}
 t_x &= 0 \\
 t_y &= 0 \\
 t_z &= 1.0
\end{align*}
$$

at $z = 30$.

Torsion:

$$
\begin{align*}
 t_x &= -0.1 \sin \theta \\
 t_y &= -0.1 \cos \theta \\
 t_z &= 0
\end{align*}
$$

at $z = 0$ and

$$
\begin{align*}
 t_x &= 0.1 \sin \theta \\
 t_y &= 0.1 \cos \theta \\
 t_z &= 0
\end{align*}
$$

at $z = 30$.

with units of MPa, so that the traction vector $t = (t_x, t_y, t_z)$.

3.2.1. Tube without side holes—tension loading. For the ‘as-built’ tubes shown in figure 5, the von Mises stress for each condition under a nominal tensile stress of 1 MPa is shown in figure 7 for the outer surface of each tube. The homogenous elastic response with no microstructure is shown in the left-most image of figure 7 for reference. Between grains, stress variations observed are on the order of ±50% with smaller stress variations within a single grain. As scan speeds increase (leading to smaller grain sizes), the local stress fields become increasingly diffuse. As shown in figure 5, at 8 mm s$^{-1}$, elongated grains remain at the mid-surface of the tube wall, despite the outer surfaces being populated by fine, more equiaxed grains. The von Mises stress for this microstructure displays two scales of response. First, there is variation between each exterior grain, and secondarily, the influence of the large interior grains through a banded helical pattern is apparent. This large-scale banding is most pronounced in the 4 mm s$^{-1}$ condition. Contrastingly, for speeds of 10 mm s$^{-1}$ and faster, this underlying longer-range behavior is eliminated. This suggests the existence of a threshold value relative to grain size that allows or eliminates a long-range stress response. This is due to the decrease in grain size which in turn reduces the clustering of similarly-responding material volumes. As these randomly assigned grain orientations are sampled, they are samples in a greater quantity per volume due to their decrease in average size.

Figure 7 shows the tensile response for one microstructural instantiation at each scan speed. However, the specific microstructures resulting from an AM build, whether obtained by experiment or by these simulations, are inherently stochastic. While general trends can
often be extrapolated, small fluctuations during the solidification process result in unique microstructures for each build. With proper process control, experimental microstructures that are near statistically equivalent could be produced. However, even with effective process control, some level of variation is expected even with identical processing conditions.

To demonstrate the inherent variation within even a statistically equivalent microstructure, three unique microstructural instantiations (obtained by exercising a unique seed value within the kMC random number generator) at each of the four previously prescribed scan speeds; 4, 8, 10, and 16 mm s\(^{-1}\), underwent DNS simulation. Each instantiation across all scan speeds maintained their overall grain size and morphological distributions, but possessed local variations to initial grain membership and grain neighborhoods. To compare the results of each instantiation, a line scan of the von Mises effective stress was performed along the length of each tube at each simulation condition and are shown in figure 8. The stress magnitudes shown on the vertical axis is calculated as the Frobenius norm of the stress tensor. The homogenized tube’s response (shown as a dashed line) is uniform along the tube’s length as expected for the simple tension loading. The plots reveal that the periodicity of the stress response is significantly influenced by the grain size. The oscillations in the stress response increase in frequency with decreases in grain size while the magnitude of variation from the homogeneous response is typically constrained between ±50% across all cases.

3.2.2. Tube with side holes—tension loading. In order to simulate the presence of a stress concentration in the tube, a hole was ‘machined’ into the simulation volume. The circular hole was aligned transverse to the length of the tube and was centered at the midpoint of its length (see figure 2). As a baseline, elasticity simulations were performed on a hole-drilled tube absent of microstructure possessing homogenized material properties. The result of this baseline simulation is shown in the left plot of figure 9.

The microstructures used in section 3.2.1 were then used in DNS simulations of the machined tubes. The resulting stress fields are shown in figure 9. In comparison to the
homogenized case, the stress state is similar but again significantly influenced by the local grain size. The influence of the microstructure is observable in the response, but the volume retains the overall response pattern as seen in the homogeneous tube with low-stress regions aligned near the hole in the direction of the tube’s length. The high-stress regions emanate at 45° from the hole and form a diamond pattern around the tube’s circumference.

Figure 8. Line scans of von Mises stress for three microstructural realizations at four scan speeds for a tube in tension (no side holes). The homogenous response is indicated as a dashed line.

Figure 9. Von Mises stress field from DNS simulations of tension loading of tubes with side-hole for microstructures simulated at four scan speeds. The homogeneous response (resulting from no microstructure) is shown at the left. Here, the full simulation domains are shown (i.e. outer-most wall thicknesses).
As seen by comparing figures 7 and 9, the imposition of a hole in the tube wall results in a more complex stress state than a uniform tube. As in figure 8, line plots are used to demonstrate the stress response for the homogenized case and compared with three unique instantiations across the four kMC simulation conditions. For the tube with side holes, the highest stresses are observed along the machined hole’s edge. Therefore, unlike figure 8, line scans are returned along a curve immediately around the hole. Figure 10 shows the response of three microstructural realizations at each condition. As in figure 8, the homogeneous response is indicated by a dashed line. Microstructure-dependent stress variation remain within a \(\pm 50\%\) range relative to the local homogeneous response. However, the absolute magnitude of the variation is much higher than that shown in other regions of the tube (due to a larger magnitude of the mean response). Localized microstructure-dependent responses reach nearly seven times the minimum magnitude of the baseline response. This supports the notion that even in relatively well-behaved microstructural arrangements, extreme value behavior precipitated by local microstructure can be significant in the vicinity of a stress-concentrating feature within the part geometry [41].

3.2.3. Tube with side holes—torsional loading. To explore the effect of microstructure under a more complex loading state, the machined tubes used in the previous section were also studied under torsional loading. The homogenous stress field is shown in the left-most image of figure 11. As with the case of tension loading, the introduction of microstructure creates a locally heterogeneous response which, to varying degrees, maintains the long-range macro-response observed in the homogenized case. The four microstructures show increasing extensions of the high stress regions along the length of the tube with lower scan speeds.

Line scans were again performed along a curve around the side hole for the torsional load case. The resulting plots are shown in figure 12. As can be observed, departures from the homogenized case vary in the \(\pm 50\%\) range for each of the three instantiations observed while...
Figure 11. Von Mises stress field from DNS simulations of torsion loading of tubes with side-hole for microstructures simulated at 4 scan speeds. The homogeneous response (resulting from no microstructure) is shown at the left. Here, the full simulation domains are shown (i.e. outer-most wall thicknesses).

Figure 12. Line scans of von Mises stress around the side hole under torsional loading for three microstructural realizations at four scan speeds. The homogenous response is indicated as a dashed line.
the frequency of oscillation surrounding the nominal stress response increase with increasing scan speed.

3.3. Fourier analysis of DNS response

By examining the stress magnitudes in spatial-frequency space across each scan speed scenario presented above, the strength of variability associated with each mechanical response can be analyzed in more detail. In figure 13, the DFT of stress magnitudes for all DNS realizations are shown. The DFT results were calculated on a trace parallel to the z-axis at $x = 0, y = 4.125$ mm (the same trace shown in figure 8). Each column contains results for a certain loading condition (e.g. tension, tension-with-hole and torsion-with-hole), while each row corresponds to a specific scan speed (4, 8, 10, and 16 mm s$^{-1}$). As shown in the leftmost images of figures 9 and 11, the homogenous response of the tube-with-side hole geometry varies spatially for both tensile and torsional loading cases. This variation produces additional DFT peaks at low frequencies. In order to isolate only the microstructure-dependent response, the homogeneous tube’s response is subtracted from the microstructure-dependent realizations for columns (b) and (c) before calculation of the DFT.

At the slowest scan speed, low spatial frequencies in stress dominate, but decay in magnitude at increasing spatial frequencies. As scan speed increases (and grain size decreases), the peaks at low frequencies decreases, and the DFT results are increasingly uniform across frequencies. This suggests that the greater the grain size, the more locally isolated the departures from a homogenized mechanical response are. This is corroborated by
the von Mises line scans in the upper left of figures 8, 10 and 12 which show near equal-value departures from the nominal homogenized result but display a much lower frequency content than those associated with the smaller grain sizes produced at higher scan speeds. These results show a characteristic length scale in micro-scale mechanical response can be readily observed in simulation and that it is influenced by the length scale of the local microstructure.

4. Discussion

4.1. General observations

With respect to processing’s impact on microstructure, the simulation parameters used in this relatively constrained study spanned the columnar-to-equiaxed microstructure transition. Even when imposing a constant molten pool shape across all cases, the transition between microstructural grain morphologies occurs over a relatively small range of a single simulation input, and by extension, a relatively small range of a physical processing parameter. This observation is consistent with the highly constrained and very abbreviated ‘mixed’ region observed in many $G/V$ diagrams denoting resulting grain morphology types under specific pairings of thermal gradient and solidification front velocity [4, 51]. A closer inspection of the parameter space utilized in this study demonstrates that finer, equiaxed grains appear at the wall midpoint among the elongated grains at a scan speed of 8 mm s$^{-1}$. At a scan speed of 10.8 mm s$^{-1}$ the elongated grains (defined here as grains spanning several build layers) were eliminated from the simulation domain completely. These results demonstrate the sensitivity of the AM process near the transition threshold. Many builds are also susceptible to variations in $G/V$ during the build process, due to changing boundary conditions (e.g. distance from a heat sink, bulk versus surface thermal history, radiative cooling environments, near part-to-part build proximity, and many others). This can be beneficially used to control local microstructure [51] but will at a minimum require thoughtful consideration for complex geometries with and without thin walls where variable cooling conditions will likely influence local microstructural arrangements.

With respect to the impact of microstructure on mechanical response, this study suggests that even within the elastic regime, microstructure can induce a significant local variation in the stress response of AM builds. Furthermore, this study shows that these variations may be significant enough to be considered when performing macroscopic simulations of mechanical response, particularly in cases where wall dimensions can approach the length scale of large AM grains.

4.2. Implications for PSP linkages and AM modeling

This study presents an example of developing a simulation linkage between processing, resultant microstructure and mechanical performance. Given the rapidly developing but thoroughly expansive design space for AM, such a workflow is highly desirable for the potential savings such a workflow can provide in time, materials or labor realized by computational exploration of a design space [52]. The high-fidelity models here required over 1000 CPUs per computation (to satisfy memory requirements), making them uneconomical for small companies hoping to quickly implement AM in their production process. However, this class of detailed simulations can serve as the basis for error-estimation procedures, early prediction of performance tolerances for as-built AM components or processes, and geometry parameter exploration for examination of feasible and unfeasible designs.
Additionally, an important issue for the modeling of mechanical performance of AM materials is the identification of RVE or statistical volume elements (SVE) and whether or not these approaches can sufficiently capture the response of AM material. The importance of this issue is emphasized by the often-promoted capability of AM methods to produce complex, non-traditional structures [53, 54]. These structures often result in thin-sections and walls that have greater sensitivity than bulk material to variations in build parameters and resultant microstructure or performance [55]. Therefore, as shown here with these idealized examples, unless stochastic variability is robustly built into the establishment of an RVE or SVE, they may not be well suited to current as-built AM materials. Furthermore, the extreme value or tails of mechanical response distributions in AM material may likely elude capture in traditional RVE or SVE domains as they will most likely result from the confluence of predictable subsets, combined with larger length scale factors such as an irregular geometry, a stress concentration, porosity, AM build support structures, build plate removal machining, surface oxidation or other such items. To this end, many non-traditional geometries are designed using topology optimization algorithms [53]. Due to computational constraints, these methods often assume isotropic, homogeneous material properties. The mechanics simulations shown here suggest this level of understanding is important to generate tolerances for material properties whether the final geometry is topologically optimized or not.

4.3. Future workflow improvements

Although the current simulations demonstrate process-parameter influenced microstructural variation and resulting material behavior, there are several viable next steps for improved model fidelity and accuracy. First, a non-trivial approximation in the simulations shown is the use of the same molten zone geometry for all scan speeds. Experiment and thermofluid simulation have both shown scan speed in welding and AM can be correlated to the general melt pool size and shape, and that melt pool dimensions are strongly influenced by surface tension through the Marangoni effect [56–60]. With increasing speed, molten zones generally become shallower and more elongated in the scanning direction. At low speeds, molten zones are significantly deeper and truncated along the scanning direction. For very low speeds or very high beam powers, vaporization of material can also occur and result in keyhole formation and intermittent keyhole collapse [61–64]. A uniform molten zone geometry will not recreate or capture these periodic perturbations. As such, a more rigorous melt pool description would eliminate the need for an idealized static geometry and may yield to more appropriate and accurate individual grain morphologies on a local level. However, selection and implementation of a model is non-trivial as it is desired that any such model would not impinge on the current framework’s ability to produce rapid, computationally efficient, and large build-scale predictions of AM microstructures.

Second, many AM builds exhibit crystallographic textures, with large columnar grains often having a fiber texture along their extended axis and coinciding with the build direction. In future work, these textures could be adapted either through statistical mapping from experimentally-acquired orientation distributions, or from the incorporation of a physically-relevant solidification model in the kMC framework. Microstructure prediction tools based on the cellular automata solidification model [12, 15] can generate texture predictions and are reasonable goals for implementation. However, work is needed to optimize these methods for the generation of large-scale AM microstructures.

The current synthetic microstructures also lack porosity defects, which can be produced in AM processes by lack-of-fusion, trapped porosity, and/or keyhole collapse [65, 66]. Materials created by un-optimized processes can demonstrate stochastic failure driven by
residual porosity [67, 68]. Even after optimization, many processes can still result in non-negligible pore fractions [65]. Post-processing methods such as hot isostatic pressing are capable of significantly reducing the pore fraction however, complete elimination of porosity is not guaranteed. The inclusion of relative amounts of porosity as is observed experimentally may be a useful activity to pursue.

Lastly, with the proliferation of AM methods in commercial applications, enhanced temperature dependent crystal plasticity material models are needed. These models are needed to account for the non-morphological microstructural characteristics found in AM builds, such as solute segregation during solidification, varying dendrite morphologies, porosity from lack-of-fusion or trapped gas defects, and impurities resulting from the build. At present, treatments of these highly complex and challenging phenomena are largely absent from material models seeking to describe and predict response among the rapidly developing field of additive manufacturing. Future work will explore behavior in the plastic regime using a crystal plasticity model as described in Bishop et al [23], incorporate as-solidified crystallographic textures, and include a non-local model to describe grain size effects [69].

5. Conclusions

The work presented here utilizes 3D synthetic metal additively manufactured microstructures as inputs for DNS of the mechanical response. Simulations were confined to the elastic regime but show tremendous promise for computationally linking processing parameters to microstructure and exploration of said microstructure’s mechanical performance. Comparisons were made to the homogenous response. The results presented here demonstrate the following:

- Local microstructure can induce significant variations on the order of ±50% from the baseline homogenized response and up to seven times the domain’s minimum stress in the most extreme case explored here.
- The frequency of oscillation of these local variations in stress was observed to be highly dependent on grain size, as most variations occurred between grains.
- Conversely, the magnitude of variation in mechanical response was largely independent of grain size with every instantiation having similar minima and maxima at ±50% of the homogenized response.
- While the overall, long-range macro-response of the simulated volumes were similar across nearly all cases, the impact of the underlying microstructure appeared more dominant in cases of large columnar grains whether present only internally or throughout the entire wall thickness.

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ORCID iDs

Theron M Rodgers © https://orcid.org/0000-0003-0440-3985

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