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Simulation of metal additive manufacturing microstructures using kinetic Monte Carlo

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ABSTRACT

Additive manufacturing (AM) is of tremendous interest given its ability to realize complex, non-traditional geometries in engineered structural materials. However, microstructures generated from AM processes can be equally, if not more, complex than their conventionally processed counterparts. While some microstructural features observed in AM may also occur in more traditional solidification processes, the introduction of spatially and temporally mobile heat sources can result in significant microstructural heterogeneity. While grain size and shape in metal AM structures are understood to be highly dependent on both local and global temperature profiles, the exact form of this relation is not well understood. Here, an idealized molten zone and temperature-dependent grain boundary mobility are implemented in a kinetic Monte Carlo model to predict three-dimensional grain structure in additively manufactured metals. To demonstrate the flexibility of the model, synthetic microstructures are generated under conditions mimicking relatively diverse experimental results present in the literature. Simulated microstructures are then qualitatively and quantitatively compared to their experimental complements and are shown to be in good agreement.

1. Introduction

1.1. Metal additive manufacturing techniques

Metal additive manufacturing (AM) allows for the creation of non-traditional and highly complex parts with sophisticated geometries [1]. The field is rapidly evolving with significant activity directed toward improving processing methods, understanding material compositions, developing post-build heat treatments, and the computational tools to treat these various aspects [1–4]. Based upon the powder-delivery method, metal additive manufacturing methods can be classified into two general categories: (1) Laser Engineered Net Shaping (LENS) or (2) Powder Bed Fusion (PBF). LENS methods utilize a carrier gas stream to transport powder through a nozzle directly into a melt pool (typically generated by a coaxial laser) at the surface of the build [5]. In PBF, a heat source (typically an electron or laser beam) is rastered across a bed of metallic powder to locally melt and solidify material. Upon completion of a layer, additional powder is spread onto the bed from an adjacent reservoir [6] and the process continues. Both methods construct builds in a layer-by-layer fashion, but have markedly different melting and solidification dynamics. Raster-patterns in LENS methods are typically less complex than those found in PBF, as the powder nozzle and coaxial laser assembly must move in tandem. Alternatively, PBF techniques, which raster the incident beam with mirrors or electromagnetic fields, are capable of faster scan rates and more elaborate scan strategies [7,8].

1.2. Common features of AM microstructures

While metal additive manufacturing techniques can be generally classified in two categories, the multitude of machines, material systems and specific goals for AM implementation have yielded tremendous variety in microstructures. This drastic variability at the microstructural level is due to the non-uniform local solidification behavior occurring in the process [1,2]. Common features of the resulting heterogeneity are a mixture of elongated and equiaxed grains, often having a visible periodicity corresponding to the layer height, line width and scan pattern used [7,9]. The transition between these grain types is controlled by the thermal gradient (G) and solidification front velocity (V) at the solid-liquid interface. These two parameters have been used to understand

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and predict microstructural morphologies in directional solidification [10] and welding for decades [11,12].

In addition to basic solidification behavior, the varying scan patterns for PBF and LENS methods have also been shown to produce significant changes in grain structure [7,9]. Island scan strategies in PBF (where the build layer is divided into independently-scanned sub-regions) can lead to rectangular partitions of elongated grains bound by equiaxed microstructures [7]. Linear scan patterns in LENS can lead to more continuous grain structures along the scan direction [13]. Furthermore, simple variations such as scanning in a uni- or bi-directional pattern, or cross-hatching between layers can also lead to additional variation in resulting grain morphology [9,14]. These deviations from microstructures created by traditional techniques can result in varied mechanical properties [15–17]. The variation across such an extensive and sensitive set of processing parameters makes the use of traditional design of experiment approaches both expensive and time consuming. However, the use of process modeling and subsequent data science based analyses offer a significant opportunity for the acceleration of process development and microstructural forecasting in the realm of AM [18].

1.3. Applications of computational materials science to AM

Current models for microstructure prediction in additive manufacturing are often extensions of methods initially developed for directional solidification or welding [19]. A number of these have included coupled cellular automata-finite element (CAFE) [20–24] or Lattice Boltzmann-cellular automata approaches [25,26]. The cellular automata models were designed for a single solidification front with limited effects from subsequent reheating or remelting. Additionally, while these methods often simulate grain growth with a detailed treatment of solidification, most are currently limited to two-dimensions and/or a relatively restrictive number of heat source passes in comparison to an actual additive build. Comparisons of the strengths and weaknesses of these various methods are summarized in Table 1. It is important to note that for current computing capabilities, even "low" cost methods may remain impractical for microstructural simulations of an entire AM build (especially for powder-bed methods where the cumulative path length of the beam over the entire build process can be many kilometers [4]).

The need for computationally efficient techniques to predict varying characteristics of AM-produced components, at the scale of experimental builds, has been identified by many researchers [3,25,27]. This is a challenge as typical additive manufacturing processes can require solidification of hundreds of layers and hours of build time. Many electron-beam and laser welding models capture relevant physics but are limited to short lengths and/or abbreviated time scales [12,28]. Current literature suggests a number of simulation methods are under active development for either high-fidelity modeling of AM processes at short times and small length scales [27], or conversely, lower-complexity simulations at longer times and greater length scales [29,30]. Regardless, few methods exist that capture fine-scale microstructural detail across a sufficiently large scale to predict microstructure over many passes and layers.

In the 1980s Ashby, Easterling, and Ion proposed a kinetics-based model for the prediction of average grain size in the heat-affected zone (HAZ) of weldments using a formalization of stochastic probability [32,33]. This model argued that curvature-driven grain growth within a thermal gradient was the dominant mechanism for grain evolution. The kinetic model used closely resembles the integration of the Metropolis function (commonly used in many Monte Carlo simulation techniques) over the temperature history present. Recently, Wang, Palmer, and Beese extended the model to predict average grain size in AM microstructures [15]. Although the mechanism of grain nucleation from the molten zone has yet to be robustly treated in models of this fidelity, these works show significant portions of grain formation can be reliably described by the treatment of grain boundary curvature as a primary mechanism.

In this work, a similar approach is invoked for the simulation of grain evolution over hundreds of passes in a 3D domain. The method is derived from the Potts kinetic Monte Carlo model for grain growth [34] and builds upon recent modifications to enable

Table 1
Comparison of AM microstructure simulation methods.

Method and Approximate Computational Cost	Benefits	Challenges
Cellular Automata-Finite Element (CAFE) (High) [21,23]	• Provides coupled predictions of thermal behavior and microstructure. • Incorporates crystallographic texture.	• Does not simulate solid-state grain evolution after solidification. • Limited to few passes of a heat source. • Free open-source code currently unavailable.
Cellular Automata-Lattice Boltzmann (High) [26]	• Allows for coupled thermofluid and microstructure evolution on same lattice. • Incorporates crystallographic texture.	• Lattice Boltzmann provides unstable solutions for many regimes. • Does not simulate solid-state grain evolution after solidification. • Limited to few passes of a heat source. • Free open-source code currently unavailable.
Monte Carlo (Medium) [18,30]	• Predicts full 3D microstructures with hundreds of heat source passes. • Approximates microstructure during solidification and solid-state grain evolution. • Utilizes idealized molten zones, without the need to parameterize for specific material systems. • Included in the open-source SPPARKS Monte Carlo suite.	• Does not allow for direct coupling of thermal and microstructural models. • Quantitative ties to experimental conditions are less developed. • Currently does not incorporate material texture or anisotropy.
Empirical Microstructure models (Low if thermal prediction exists, otherwise medium) [31]	• Estimates microstructural features over large builds. • Allows extension of pre-existing thermal simulation models.	• Does not provide microstructure for further analysis. • Requires estimation of thermal environment. • Not well explored for many material system in AM.