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Understanding grain evolution in additive manufacturing through modeling

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ABSTRACT

Variability in the mechanical properties of additively manufactured metal parts is a key concern for their application in service. One of the parameters affecting the above-mentioned property is solidification texture which is driven by scan patterns and other process variables. Understanding of how these textures arise in the AM process can provide a pathway to control these features which ultimately decide the final structural material properties. In this work, a Cellular Automata (CA) based two-dimensional microstructure model is formulated and implemented to understand grain evolution in AM. Grain evolution in multilayer depositions using various scan patterns in Directed Energy Deposition (DED), Metal Laser Sintering/Selective Laser Melting (MLS/SLM), and Electron Beam Melting (EBM) is presented and qualitatively compared with reported literature. Results show strong correlation of scan patterns with evolving grain orientations. Variability in grain size and orientation evolution during SLM and EBM processing of metallic materials showed direct influence by exposure to different cooling rates and thermal gradients. The similarities between the simulated and reported results lead us to conclude CA based modeling for predicting grain orientation and size in metal AM processes is useful for prediction of continuum level structural properties at global and local length scales.

1. Introduction

Metal based additive manufacturing (AM) processes are some of the most promising manufacturing routes for producing near net shape metallic products. Advantages of AM over conventional manufacturing technologies include greater flexibility for generating complex geometries with less lead times and raw material consumption [1–3]. Based on the input feed system and energy source, the metal melting-based AM methods can be broadly classified into Directed Energy Deposition (DED), Selective Laser Melting (SLM), and Electron Beam Melting (EBM). Detailed information about each machine, their feed system and energy source can be found in literature [4].

The main challenge in the adoption of AM technology is the qualification and certification of parts [5]. For qualification, a part must be built without failure and should possess mechanical properties above a certain specification for it to fulfill its service requirement. The mechanical property of any AM part is derived from its solidified microstructure features such as grain size, grain type, texture, and present phases [2]. Variability in the microstructure due to different process conditions generates non-uniform mechanical property variations in a part [6,7] which limits its predictability and qualification. Common variability in the microstructures are the types of grain (such as equiaxed or columnar) driven by thermal gradient (G) and solidification rate (R) [8–10], texturing due to use of various scan patterns [11–15], and deleterious phase formation [16,17] during cooling. Identification of the above-mentioned variabilities and their correlation with mechanical properties through experimental routes is a tedious process which requires a large set of experiments. This not only extends the qualification time but also requires a huge amount of resources and money. With the help of predictive tools, these variabilities could be simulated and the outputs could be further used for the estimation of mechanical properties before the part is printed. This eases the decision making as the process parameters suitable for achieving desirable properties could be rapidly chosen in addition to saving time, money, and resources.

Various works [18–23] have been published which predict AM material microstructures. Most of these works are a direct adoption of welding process predictions, which resemble AM; however, AM is more complicated, considering rapid high heat input and repeated heating and cooling cycles. Phase field [18,19], Monte-Carlo [20], Stochastic analysis [21], and Cellular Automata [22,23] methods are commonly used for the simulation of these features in AM processes. Among these methods, the Phase field method is often considered the most accurate method followed by Cellular Automata and other methods. The downside of using the Phase field method is its computational cost; and therefore, these methods are limited to small size scales. On the other hand, Cellular Automata methods have a good tradeoff between accuracy and scalability for large domain sizes. When it comes to AM, small-

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scale features such as segregation and deleterious phase formation do matter, but large-scale feature such as texturing due to scan patterns also matter. The development of texture in AM processed parts gives rise to anisotropic mechanical properties. Therefore, prior prediction of anisotropy is of paramount importance to evaluate mechanical property evolutions in AM parts.

Wei et al. [15] performed numerical heat transfer and flow calculations to provide understanding of solidification morphology and texture development in multi-layer AM processes for unidirectional and bidirectional scanning. Their work provides aspects of texture development in multi-layer AM but only shows a schematic representation of texture, mapped using maximum heat flow direction. Recently, Rodgers et al. [20] at Sandia National Laboratories captured 3D grain evolution of solidified structures using a Q-Potts Monte Carlo approach. Their work widely showed different types of texture and grain evolution in AM driven by various scan patterns. However, the model does not include the direct influence of thermal gradient and cooling rates on evolving microstructure as well as material texture. Simply utilizing the kinetic strength function, which is related to scan velocity, mobility, and build layers, they were able to intelligently decide what type of grains (equiaxed or columnar) are generated in the simulation domain. The advantage of using their model is that an estimation can be made of the kind of grains and their morphology. To the best of our knowledge, no Cellular Automata or Phase Field simulations are reported in literature which incorporates the effect of scan patterns on grain evolution.

In the present work, 2D-Cellular Automata was developed to simulate the grain morphology of a multi-layer build. The model incorporates the fundamental aspects of solidification to demonstrate grain evolution in AM. Effect of scan patterns, thermal gradients, and cooling rates on the resulting microstructure have been demonstrated. To save on computational time, constitutional undercooling has been neglected. Therefore, the simulation outputs grain size, type of grains, and texture information. The current model is decoupled from a thermal model and uses constant thermal gradients and cooling rates. The grain morphology results are demonstrated for different scan patterns used in AM machines and validated and discussed with the existing literature data.

2. Model description

2.1. Formulation

The Cellular Automata method is an algorithm which describes the spatial and temporal evolution of a physical system by applying deterministic or probabilistic transformation rules [24]. In this method, the spatial domain is divided into finite cells such that they can fit the simulation domain with integral multiples of the finite cell size, and the state of every cell is determined by the state of its neighbor cells according to a set transformation rule. In the present model, four variables are assigned to each cell: (a) a state variable defines the state of a cell i.e., solid, liquid, and interface; (b) an orientation variable represents the preferred growth orientation of the grain; (c) a grain number variable is used to distinguish the grains from one another; and (d) a solid fraction variable is used to track the transition of the liquid cell to solid cell. Eight nearest (first and second nearest) neighbors are selected in this model. The interface cells are identified if one of the cells at the 8 neighbor's cells is a solid cell. At the beginning, new nuclei populate at interface cells based on the nucleation law [25] (Eq. (1)):

$$\frac{\partial N}{\partial t} = -2\mu_N(\Delta T)\frac{\partial T}{\partial t}(1 - f_s) \tag{1}$$

where N is the number of nuclei, (ΔT) is the thermal gradient/total bulk undercooling, $\frac{\partial T}{\partial t}$ is the cooling rate, μ_N is the nucleation parameter, and f_s is the fraction of solid. The interface cell can represent the boundary of the melt pool and grain boundaries of solidifying grains inside the melt pool. The nucleation model incorporates the effect of both total undercooling and cooling rate. The nucleation probability of the cells located at the interface cell is calculated using Eq. (2) for every time step [25]:

$$dP = \frac{\partial N}{N^I} \tag{2}$$

where N^I is the total number of cells located at the interface (melt pool and grain boundaries). Once the probability is greater than a random number generated by the computer between 0 and 1, that cell will convert from liquid to solid. The model becomes deterministic as a function of rounding the probability variable. Once the new solid nucleus is nucleated, preferential growth direction (θ_o) is assigned based on the normal angle between the nucleated cell and the moving heat source. The driving force for growth comes from the amount of thermal undercooling present at the solid/liquid interface. The velocity of the solid/liquid interface is calculated using Eq. (3) [26]:

$$V_N = \mu_k(\Delta T) \tag{3}$$

where μ_k is the interface kinetic coefficient, and ΔT is the total undercooling that consists of thermal and curvature undercooling calculated using Eq. (4):

$$\Delta T = [\Delta T_T - \Gamma \overline{K}(t_n)] \tag{4}$$

where $\Delta T_T$is the thermal undercooling, Γ is the Gibbs Thomson coefficient, and $\overline{K}(t_n)$ is the mean curvature which is calculated according to Eq. (5) as described by [25]:

$$\overline{K} = \frac{1}{l_c}\left(1 - 2\frac{f_s + \sum_{i=1}^{N} f_s(i)}{N+1}\right) \tag{5}$$

where l_c is the size of the cell and N is the total number of neighbor cells including both first and second nearest neighbors sharing the edge and corner of the given cell. In this case, that number is 8. To account for anisotropy, the crystal growth velocity (V_g) according to the crystal preferential growth direction (θ_o) is calculated using Eq. (6):

$$V_g = V_N\{1 + \delta_k \cos[4(\theta - \theta_o)]\} \tag{6}$$

where δ_k is the degree of kinetic anisotropy and θ is the angle between the horizontal direction and the normal to the solid/liquid interface. The angle θ is obtained from the gradient of solid fraction at the solid liquid interface. Once the velocity of the interface is obtained, the rate of change of the evolving solid fraction at the interface cell is calculated using Eq. (7):

$$\Delta f_s = G\frac{V_g}{l_c}\Delta t \tag{7}$$

where Δt is the time increment and G is a geometric factor related to the first and second nearest neighbors. G is calculated using Eq. (8) as described by [26]:

$$G = 0.4\left(\sum_{n=1}^{4} b_n^I + \frac{1}{\sqrt{2}}\sum_{n=1}^{4} b_n^{II}\right) \tag{8}$$

where b^I and b^{II} represent first and second nearest neighbors respectively in a square grid. The geometric factor accounts for higher solidification rate for first nearest neighbors compared to second nearest neighbors. If the fraction solid of a cell becomes 1, the status of a cell changes from an interface to a solid cell. The simulation runs until all the liquid cells change to solid. The constants used for this simulation are as follows: lattice size (l_c) = 1 μm, interface kinematic coefficient (μ_k) = 2×10^{-6}, Gibbs Thomson coefficient (Γ) = 1.7×10^{-7}, degree of kinetic anisotropy (δ_k) = 0.7, and nucleation parameter (μ_N) = 10^3.