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Three-dimensional modeling of the microstructure evolution during metal additive manufacturing

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ABSTRACT

Prediction of microstructures of additive manufactured materials is a significant research focus to face the challenge of producing tailored components. In this work, a three-dimensional numerical model is developed to evaluate fundamentals of grain structure evolution during metal additive manufacturing. Cellular automata and finite difference methods are coupled to predict the grain structure, depending on a transient temperature field during the additive manufacturing process. Selective laser melting process that makes use of a high energy density laser beam to produce parts of highly complex shape by melting of metallic powder is examined. The predicted grain structure is consistent with the experimental data. The results obtained show that specific solidification conditions in selective laser melting and grain selection associated with competitive nature of grain growth promote the development of coarse columnar grains with the most favorable growth direction misaligned with the build direction. This results in morphological and crystallographic texture.

1. Introduction

Additive manufacturing (AM) demonstrates very high rate of development, and manufacturing of metal parts is one of the fastest growing applications of AM [1]. The majority of metal AM systems worldwide utilize a powder bed fusion process [1,2]. In the framework of this process, a heat source scans the selected locations of the powder bed at the controlled rate and melts the powder which then solidifies as it cools to form a first solid layer of the part to be produced. The first powder layer is applied on a substrate fixed on the building platform. Then the part is produced in a layer-by-layer fashion. The heat source can be either a laser (selective laser melting or SLM) or an electron beam (selective electron beam melting or SEBM).

Microstructure formed during the manufacturing process is one of the key factors defining the mechanical properties and application of a material. Microstructure and, consequently, mechanical properties of parts produced by metal AM and conventional methods are known to be considerably different [2,3]. A strong morphological and crystallographic texture is observed in additive manufactured specimens [2–12]. Strength and ductility are shown to differ when loading is parallel and perpendicular to the build direction [2]. The large columnar grain boundaries are reported to be preferred regions for crack propagation [10,11]. Characteristics of a material microstructure such as grain size, grain shape, grain orientation are complex functions of process parameters. It is reported that there are more than 130 parameters that could affect the SLM process [13]. Scanning speed, beam power, scanning strategy, hatch distance (scan-line spacing), and thickness of powder layer are considered as the principal parameters in SLM [14]. Yet optimum process parameters are chosen empirically which is an expensive and time-consuming exercise.

Computational modeling is an attractive tool for a comprehensive study and optimization of material properties of additive manufactured material. To date, the overwhelming majority of theoretical works have been focused on physics-based process simulations for the metal AM, aimed at analyzing temperature and velocity fields and residual stress accumulation on the macroscopic scale (see, for example, [15–19]). Modeling of the AM-induced microstructure evolution is becoming a hot topic and beginning to emerge in the literature.

Let us briefly review the efforts of grain growth simulations for metal AM. Rai et al. [20,21] created a two-dimensional (2D) cellular automata (CA) lattice Boltzmann (LB) model accounting for powder related stochastic effects, energy absorption and evaporation, melt pool dynamics and microstructure evolution. The 2D CALB model was applied to study the effect of process parameters (hatch distance, scanning speed and strategy) on the evolution of grain structure, induced by SEBM in a nickel-based superalloy. Rolchigo

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et al. [22] worked out a 2D multiscale model coupling a macroscale description of beam melting problem with a microscale CALB model to describe a specific AM process, Laser Engineered Net Shaping (LENS™), on the scale of individual dendrites. For the process modeling on macroscale, use was made of the fluid flow and heat transfer modules of COMSOL Multiphysics. Panwisawas et al. [23] accounted for powder size distribution, melt flow, evolution of grain structure, and γ'' precipitation in the framework of a three-dimensional (3D) OpenFOAM computational fluid dynamics (CFD) cellular automata-finite element (CAFE) model. The proposed microstructure-based modeling approach aimed at prediction of the behavior of laser-powder interaction, surface structure, porosity development and evolution of grain structure during SLM of a nickel-based superalloy IN718. A 3D FE model constructed by Marion et al. [24] to simulate direct metal deposition (DMD) process did not take into account grain structure explicitly but enabled the phase transformations developing in Ti-6Al-4V to be analyzed. Zhang et al. [25] and Lopez-Botello et al. [26] simulated metal AM of titanium and aluminum alloys, respectively, with the use of CAFE models based on the approach put forward by Rappaz and Gandin [27]. In both cases, the CA models adopted to describe the mesoscopic morphological evolution were two-dimensional. Nie et al. [28] offered a stochastic FE model to reproduce dendritic microstructures of an Nb-bearing nickel-based superalloy under the conditions expected in SLM solidification. However, the developed model suffers from artificial anisotropy caused by the mesh. In other words, the main propagation axes of the simulated dendrites are aligned with the global coordinate axes and exhibit the same orientation. Sahoo and Chou [29] simulated the dendritic growth during SEBM with the use of phase field model. However, since the phase field method takes considerable computing power, the dendrite growth simulation was limited to a single grain. Recent progress has also been reported for the 3D simulations of grain structure evolution during metal AM with the use of Monte Carlo (MC) technique [30]. The benefits of MC simulations are sufficiently low computational costs and thus ability to predict 3D microstructures with hundreds of heat source passes. Although the kinetic MC model allows grain morphology to be described, yet it does not incorporate a crystallographic texture of additive manufactured material.

Most models mentioned above focus on the physical phenomena occurring locally in the melt pool (fluid flow, Marangoni effect) [20–23] or describe complex dendritic structure [22,28,29] but due to the high computational costs, simulation of multiple passes of a heat source is challenging. Other models (see, for example, [24]) enable AM of industrial parts to be simulated but cannot provide microstructural data for analysis and further applications in mechanical calculations.

While extensive experimental studies on additive manufactured microstructures have been performed, the nature of microstructure formation is still not fully understood and the mechanisms involved have yet to be investigated. An important task necessary for understanding of the final microstructure is deriving of its dynamic evolution during solidification. Currently it is numerical simulations which make it possible. Up to date most of the calculations of the microstructure evolution induced by AM are performed in a 2D formulation [20–22,25,26,28,29,31,32]. Analytical review of the literature on the subject indicates that there is a considerable gap in 3D numerical studies on the evolution of grain structure during metal AM. Moreover, due to high computational costs, it is a single pass of heat source that has been simulated in the 3D setting. The results obtained in these simulations give no way to see the full picture of microstructure evolution induced by metal AM. Real materials are three-dimensional, and microstructural effects are three-dimensional as well. Three-dimensional formulation of the problem is of particular importance in the case of a relatively deep melt pool. When the resulting melt pools are deep, the impingement effects of a large number of columnar grains oriented in three dimensions play a vital role in the formation of final microstructure [21,31].

In this communication, we report the evolution of polycrystalline structure during metal additive manufacturing. For this purpose, we developed a 3D CAFD model accounting for the interrelationship between processing and microstructure. The 3D numerical model combines the modified CA approach developed by Rappaz and Gandin [27] and the FD solution of the heat transfer equation. The evolution of grain structure in a specimen subjected to SLM is simulated. We consider not an entire part but a subvolume in the form of a rectangular cuboid. Conclusions regarding the kinetic, statistical, and topological aspects of the 3D grain growth during SLM processing are obtained.

2. Model description

Consider an approach to modeling of the SLM process in three dimensions. First, we need to generate a polycrystalline base plate characterized by equiaxed grains and the absence of texture. Then, the first powder layer is deposited onto the base plate. For the sake of simplicity, we use a homogenized approximation of the powder layer. The detailed physics of the process area (for example, fluid flow, Marangoni convection) is ignored to simplify and reduce the calculation time. Laser beam moves with a constant velocity according to the predefined scanning strategy. We consider the unidirectional scan vector. The scanning strategy was chosen to be identical, without rotation of the scanning direction. After each laser pass, the computational domain is cooled down to ambient temperature T^e. This is because the laser beam is assumed to go far out of the domain after each pass in the equivalent experiment. On laser irradiation of the powder layer, a new layer of powder is deposited onto the previous one. This process is repeated until a specified number of layers are built. The most widely used titanium alloy, Ti-6Al-4V, is chosen as a model material.

Although most practitioners use anti-parallel scans, not unidirectional, with tool path planning that rotates the scan axis for each layer to avoid propagation of defects between layers, it is neglected to minimize the impact of the scanning strategy on the microstructure evolution. This approach has already been used both in experimental works and in modeling (see, for instance, [33–35]) for a more detailed understanding of the processes occurring in a material during SLM.

2.1. Heat transfer

The process of transient heat transfer is described by a heat conduction equation

$$\rho(T)c_p(T)\frac{\partial T}{\partial t} = \nabla\cdot(\lambda(T)\nabla T) + Q. \tag{1}$$

Here ρ is the density, c_p is the specific heat capacity, λ is the thermal conductivity, T is the temperature, t is the time, and Q is the volumetric heat input term defined as the heat input from the laser beam. For the sake of simplicity, latent heat of fusion is not accounted for in the presented model, due to its low contribution to the heat transfer relative to the heat source effect [24,35–37]. Effects of latent heat of fusion on local thermal processes in laser welding were analyzed in detail in [38]. The shapes of melt pool and mushy zone were shown to be sensitive to accounting for the latent heat. For instance, when the rate of heat source is high, the melt pool is elongated and shaped like a teardrop. If the latent heat is neglected, given other conditions being equal, the melt pool