Computational Materials Science 153 (2018) 159–169

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Numerical investigation of effects of nucleation mechanisms on grain structure in metal additive manufacturing

Xuxiao Li, Wenda Tan*

Department of Mechanical Engineering, The University of Utah, Salt Lake City, Utah 84112, United States

ARTICLE INFO

Keywords:
Metal additive manufacturing
Multi-scale modeling
Nucleation
Solidification
Grain structure

ABSTRACT

Understanding the grain structure in metal additive manufacturing (MAM) builds is important to improve the properties of MAM builds and the controllability of MAM processes. The formation of the columnar and/or equiaxed grains in MAM are caused by an interplay of nucleation and growth mechanisms, which is numerically investigated in this work. A meso-scale Cellular Automata model combined with a macro-scale thermal model is used to predict the three-dimensional grain structure in the direct laser deposition process of stainless steel 304, with the investigation focused on the effects of the nucleation mechanisms (both the epitaxial nucleation at the fusion line and the bulk nucleation in the molten metal) on the grain structure. Our results show that the bulk nucleation condition can significantly change the grain structure (from columnar to equiaxed), and typical grain structures in MAM can be successfully reproduced using different bulk nucleation conditions.

1. Introduction

Metal Additive Manufacturing (MAM) has shown incredible capabilities to manufacture metallic parts with intricate geometries. The geometric flexibility of MAM is owing to the layer-by-layer scanning of a heat source, typically a laser or an electron beam, that melts the metal powder. A bed of metal powder is pre-deposited before the scanning of the heat source, or the metal is fed into the molten pool that is created by the scanning heat source. A wide range of metal alloys are studied in literature, such as iron-based (Stainless Steel 316L [1–3]), aluminum-based (Al-11.28% Si [4], Al-10Si-Mg [5]), titanium-based (Ti–6.5Al–3.5Mo–1.5Zr–0.3Si [6]), and nickel-based (Inconel 718 [7–9]) alloys.

The structural features of the builds by MAM can be categorized as macro-scale $\gtrsim$ 1000 μm, e.g., cracks and tears), meso-scale ($\sim$100 μm, e.g., grain characteristics, lack-of-fusion defects and trapped gas porosity) and micro-scale $\lesssim$ 10 μm, e.g., dendrite morphology and phase distribution). The characterization of these structural features is critical to understand MAM processes and helps to construct a map that links process parameters, structural features, and build properties [10]. In this paper, we focus on the meso-scale grain structure.

Despite the variety of MAM processes and metal alloys, certain characteristics of grain structure can be identified from the literature. Both columnar and equiaxed grains are observed in MAM builds. Columnar grains are commonly observed growing epitaxially from the substrate or the previously deposited layer (collectively referred as the underlying layer) and toward the scanning direction of the heat source [4,8], as shown in Fig. 1. Equiaxed grains can be found distributed among columnar grains. Ref. [9] reported an interesting "sandwich" grain structure where layers of equiaxed grains are observed between every two layers of columnar grains. In general, columnar grains are larger and have a stronger texture than equiaxed grains. Different grain morphology, size, and texture can be achieved by varying the input power, scanning velocity as well as the scanning pattern of the heat source, as widely reported in the literature [1–9].

Theories in welding metallurgy [11] can be conveniently utilized to qualitatively explain the occurrence of the above-mentioned characteristics of grain structure, as both in welding and MAM the metal material is subjected to a moving heat source with high energy input. Upon solidification, nucleation will preferably occur at the fusion line (Fig. 1) due to the lower activation energy. If the layer being built is of the same material as the underlying layer, which is often the case in MAM, the nuclei will preferably adopt the same crystallographic orientations as those of the partially melted grains in the underlying layer. This nucleation mechanism is referred as epitaxial nucleation [11].

After the epitaxial nucleation, grains will grow across the fusion line and along the local temperature gradient direction, which is approximately the local moving direction of the solidification front. This directional solidification leads to columnar grain shapes (the purple grains in Fig. 1). The grains with their certain crystal directions, e.g., the ⟨1 0 0⟩ directions for the face-centered-cubic (FCC) and body-centered-cubic (BCC) materials, better aligned with the local temperature

* Corresponding author.
E-mail address: wenda.tan@mech.utah.edu (W. Tan).

https://doi.org/10.1016/j.commatsci.2018.06.019
Received 17 February 2018; Received in revised form 8 June 2018; Accepted 9 June 2018

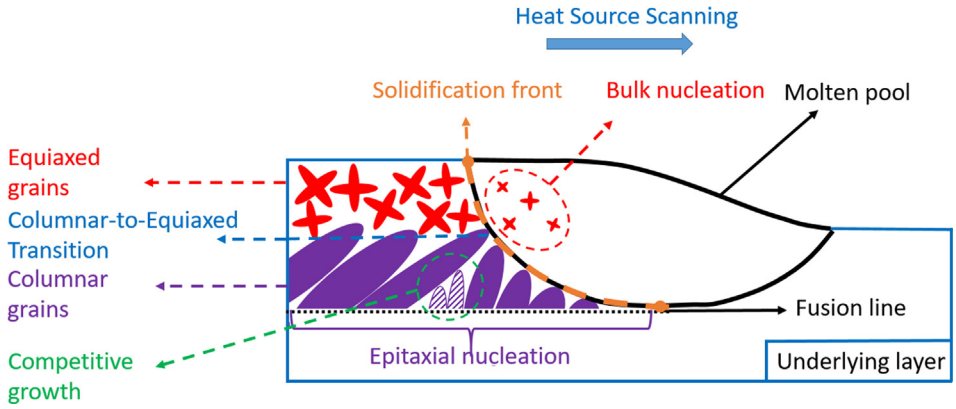

Fig. 1. Summary of possible nucleation and growth mechanisms and their effects on the grain structure in MAM processes.

gradient will outgrow the less aligned ones (such as the shaded purple grains in Fig. 1). This competitive growth mechanism [11] leads to "favored" grains dominating the grain structure, and therefore, larger grains and stronger texture can be observed, as reported in [5,12,13].

Nucleation may also occur in the molten metal ahead of the solidification front, which is referred as the bulk nucleation as opposed to the "surface" epitaxial nucleation at the fusion line (Fig. 1). The nuclei from the bulk nucleation can grow to become equiaxed grains. The equiaxed grains can coexist with columnar grains, or even stop the growth of columnar grains, referred as the Columnar-to-Equiaxed Transition or CET (Fig. 1). In literature, analytical CET models [14–16] have been used to predict the volume percentage of equiaxed grains according to the local thermodynamic conditions of the solidification front. There have been multiple studies that utilize the CET models to explain the grain structure in MAM [7,17,18]. From the above discussion, it can be seen that the grain structure in MAM is complicated by a combination of different mechanisms.

The qualitative welding theories and the analytical CET models, although having a solid physical background, cannot capture the complex scanning patterns in MAM as well as the randomness from a large quantity of grains, and thus fail to quantitatively predict the grain structure in MAM. In light of this, numerical simulations based on physical models have been recently developed to provide quantitative grain structure predictions. In literature, the Cellular Automata (CA) method [13,19–22] and the Monte-Carlo (MC) method [23] have been used to simulate the grain structure in MAM.

Following the seminal work of Rappaz and Gandin [24], several studies have shown the capability of the CA method to capture the major characteristics of the grain structure in MAM. Ref. [13,19] demonstrated the epitaxial nucleation and competitive growth mechanism in their two-dimensional (2D) models; the consequent columnar grain structure and large grain size are successfully reproduced, which are compared with experimental results. Ref. [21] extended the CA method to be three-dimensional (3D); in their multi-pass and multi-layer simulations, a strong texture resulted from the competitive growth was reported. However, these works did not include the bulk nucleation that can cause the occurrence of equiaxed grains. Ref. [20] developed a 2D model which includes the bulk nucleation; in their simulation results, the growth of columnar grains was stopped by equiaxed grains while equiaxed grains could further grow to become "new" columnar grains, which resulted in a laminar grain structure. Ref. [22] developed a similar model but in 3D version. However, only the grain structure of a single pass build is simulated. For the MC method, Ref. [23] qualitatively reproduced the columnar and equiaxed grains observed in experiments, but no detailed discussion is provided regarding the nucleation and growth mechanisms.

Based on the existing literature, it is still not well known the effects of the bulk nucleation on the 3D grain structure, especially in the complicated cases of multi-layer and/or multi-pass builds. In this work, a 3D CA model is developed that includes both the bulk nucleation and the (surface) epitaxial nucleation, and we will focus on the effects of (both bulk and epitaxial) nucleation mechanisms on the grain structure in MAM. The Direct Laser Deposition (DLD) process and the Stainless Steel (SS) 304 are chosen as a typical MAM process and metal material to demonstrate the model capability. We will describe our modeling methods in Section 2 and modeling results in Section 3. Conclusions and future works will be given in Section 4.

2. Model description

In this work, a macro-scale finite volume model is first implemented to simulate the thermal history in a DLD process. Then a meso-scale CA model is used to simulate the grain structure with the simulated thermal history as a model input.

2.1. Macro-scale thermal history simulation

In this work, we have used the common simplification in MAM modeling that the molten pool flow is ignored [25,26]. A level-set formulation [27] is implemented to implicitly capture the motion of the interface between the metal (solid or liquid) and the gas phase, which is referred as the metal-gas (m-g) interface. The level-set advection equation is written as:

$$\frac{\partial \phi}{\partial t} + F_p|\nabla \phi| = 0, \tag{1}$$

where ϕ is the level-set function. F_p is the interface velocity resulted from the powder deposition in a DLD process, which is determined by a powder flow model described in a previous publication [28]. The level-set function is defined as the signed distance to the m-g interface. As illustrated in Fig. 2, the metal phase has a negative level-set value and the gas phase has a positive level-set value; the zero-level-set iso-contour (the solid blue line) is the location of the m-g interface.

The major physics included in the current model are the heat conduction, the heat convection and radiation at the m-g interface and the thermal energy addition from the laser and the incident powder. The heat conduction equation is written in a conservative form as:

$$\frac{\partial(\rho e)}{\partial t} - \nabla\cdot(k\nabla T) = S, \tag{2}$$

where ρ is the density, e is the internal energy, k is the thermal conductivity, T is the temperature and S is an energy source term. In this work, the material properties, ρ, e, etc., are mixture properties determined by the material properties of different phases. The source term S is distributed over the m-g interface and is composed of several contributions, as given by Eq. (3)