Additive Manufacturing 13 (2017) 124–134

Contents lists available at ScienceDirect

Additive Manufacturing

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

Simulation of grain structure evolution during powder bed based additive manufacturing

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ARTICLE INFO

Article history:
Received 20 January 2016
Received in revised form 5 October 2016
Accepted 27 October 2016
Available online 5 November 2016

Keywords:
Lattice Boltzmann method
Selective beam melting
Cellular automaton
Additive manufacturing
Grain structure evolution

ABSTRACT

A lattice Boltzmann (LB) method to simulate melt pool dynamics and a cellular automaton (CA) to simulate the solidification process are coupled to predict the microstructure evolution during selective electron beam melting (SEBM). The resulting CALB model takes into account powder related stochastic effects, energy absorption and evaporation, melt pool dynamics and solidification microstructure evolution. Several physical phenomena are observed during grain solidification, e.g., initial grain selection starting at the base plate, grain boundary perturbation, grain nucleation due to unmolten powder particles in the bulk, grain penetration from the surface of the part or grain alignment dependent on the beam scanning strategy. Aim of the present work is to apply the CALB model to qualitatively examine the aforementioned phenomena. The effect of process parameters on the final grain structure and texture evolution is presented.

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1. Introduction

Powder based additive manufacturing (AM) is a technique of layer by layer free form fabrication. For metals, a laser or an electron beam are used to selectively melt the powder [1–3]. The solidification process in powder bed AM is dominated by epitaxial grain growth [4,5]. The grains grow across hundreds of layers resulting in built parts with very strong texture and anisotropic properties [4,6–8]. The resultant grain structure depends on the local thermal history and varies strongly within the component. This is due to the different heat treatment conditions within the building chamber (in situ heat treatment), which is characteristic of SEBM process. Based on applied process parameters typically the material is molten several times during SEBM. Even after final solidification, temperature of the solidified parts strongly fluctuates due to the melting of neighboring lines or subsequent powder layers. During this phase grain structure altering processes e.g., homogenization or solid state phase transformation may take place. For example, in the case of Ti6Al4V alloy built parts manufactured using SEBM, close to the top surface initial columnar β grain structure is observed. The heat affected zone may undergo solid phase transformation due to in situ heat treatment (from columnar β into $\alpha - \beta$ microstructure) [4,6,9]. Residual porosity and lack of fusion defects contribute to the formation of new grains from partially molten powder particles interrupting the epitaxial growth. The texture and grain aspect ratio in the final component are complex functions of process and material parameters [7]. The most influential process parameters are beam power, scanning speed, spacing between two consecutive beam tracks (line offset), melting strategy and return time of the beam with respect to a fixed point. For a given material and component geometry, choice of the optimum process parameters is still based on trial and error. Therefore, numerical model capable of predicting the final microstructure and texture during selective electron beam melting (SEBM) is desired.

Many different approaches have been used to simulate grain structure evolution, e.g., Monte Carlo (MC) [10], level set [11], phase field method (PFM) [12], front tracking method [13] or cellular automaton [14]. MC methods are based on the principle of surface energy minimization. They show applicability in being able to predict qualitatively the grain structure in conventional castings. However, validity of the MC simulations for grain growth during solidification is questionable, because the kinetics of the cellular/dendritic growth is not properly taken into account. PFM shows excellent capabilities for the simulation of microstructures. However, they are limited to only a couple of grains. Using PFM one system of differential equations has to be solved for each grain at every time step of calculation. Therefore, simulation of systems involving hundreds or thousands of grains is challenging due to the computational costs and capabilities. Using grain boundary tracking [13] approach, preferred trajectories of the grain growth are calculated based on analytical models for a given shape of the melt pool (approximated to standard geometrical shapes, e.g. elliptical,

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http://dx.doi.org/10.1016/j.addma.2016.10.007
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parabolic). The actual growth direction of a single grain represented by its crystallographic orientation is not taken into account and the process of grain selection is neglected. Another model based on Voronoi Diagram [15] has been reported but it is suited only for globular grain growth.

Cellular automata (CA) based algorithms describe the spatial and temporal evolution of a complex system by applying probabilistic or deterministic local rules to the cells of a lattice and the local interaction laws are formulated in terms of finite difference equations. The advantages of CA methods are their flexibility, computational efficiency and ability to capture the actual complexity to include various shapes and sizes of the grains and the tendencies typical of actual grain growth. A 2D lattice Boltzmann (LB) model has been presented by Körner et al. [16,17] to simulate powder densification, electron beam energy absorption and melt pool dynamics during SEBM. The model has been extended by a CA based grain growth model to simulate the solidification process. In the present work a 2D CALB model coupling a CA to simulate grain growth based on the model of Gandin et al. [14] and the LB model of Körner et al. [16,17], has been used to simulate solidification microstructure during SEBM. The aim of the present work is to qualitatively investigate the influence of process parameters and scanning strategy on the final microstructure of the built part.

2. Model

Fig. 1 shows all physical effects simulated by the presented CALB model. Energy transfer from the electron beam to the powder bed is calculated by taking into account powder related stochastic effects unlike the homogenized approach taken in most of the reported work in the related research fields [18–24]. Inclusion of the powder related stochastic effects is significant because net energy transfer to the powder bed is determined by the actual thermal conduction between individual powder particles which is proportional to their contact area. The wetting process of individual powder particles depends on their geometry and plays a very significant role during the consolidation process of the powder bed. Moreover, influence of gas porosity present within the powder particles (planned as future work) and grain nucleation due to partially molten powder particles on the final built part can only be incorporated into the model when individual powder particles are considered. All these effects cannot be simulated using a homogenized approach of the powder bed.

The model is based on a 2D square lattice. Thermal conduction, convection, fluid flow and grain structure simulations are also performed in 2D (*xy* plane), see Fig. 2. Electron beam movement takes place in the *xz* plane. Conservation equations employed to calculate the thermodynamic and hydrodynamic evolution are

$$\nabla \cdot \mathbf{v} = 0 \tag{1}$$

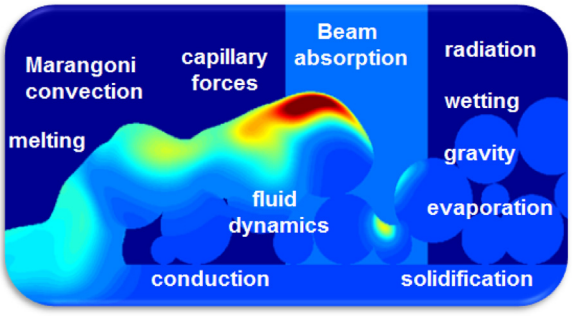

Fig. 1. Main physical effects covered by CALB model.

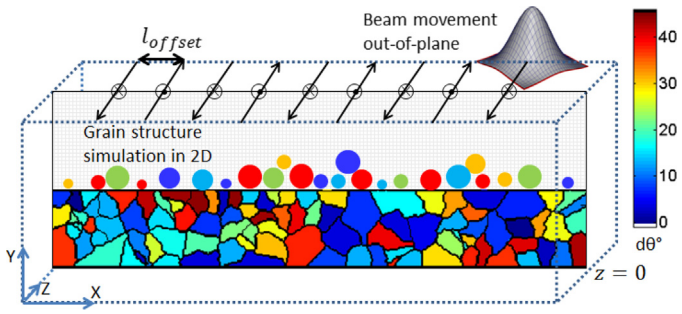

Fig. 2. CALB model initial set-up with an equiaxed base plate, powder bed and an electron beam heat source. The color bar maps the grain misorientation with respect to the build direction (*y*-axis). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article.)

$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla)\mathbf{v} = -\frac{1}{\rho}\nabla p + \nu \nabla^2 \mathbf{v} + \mathbf{F} \tag{2}$$

$$\frac{\partial E}{\partial t} + \nabla \cdot (\mathbf{v}E) = \nabla \cdot (k(T)\nabla E) + \Phi. \tag{3}$$

Here t, $\mathbf{v}$, ρ, p, ν, k and $\mathbf{F}$ denote time, fluid velocity, density, pressure, kinematic viscosity, thermal diffusivity of the material and external forces like gravity, respectively. The thermal energy density E of each cell in the lattice is given by

$$E = \int_0^T \rho\, c_p(T)\, dT + \rho\, \Delta H, \tag{4}$$

where ρ, T and c_p denote mass density, temperature and specific heat at constant pressure, respectively. The first term represents the change in energy density due to the temperature change and ΔH is the latent enthalpy of a cell undergoing a phase change. Φ is the source term for energy density conservation equation (Eq. (3)), e.g., the energy deposited by the electron beam. Since no grain movement is considered in the presented model, the solid is assumed to have a zero velocity. The conservation equations are solved using free surface LB method presented in Section 2.3.

Simulation begins with setting up a base plate with equiaxed grains (Section 2.5), followed by generation of a powder bed with specified powder bed density and powder size distribution (Section 2.1). Each cell in the simulation domain is categorized as solid, liquid, gas or interface cell. Interface cells are partially filled cells with at least one gas cell in their neighborhood and they represent the transition zone between liquid and gas phase. At the beginning all the material is in solid phase. As the beam, moving in the *xz* plane, approaches the simulation domain in xy plane, energy is transferred to the solid material causing an increase in its temperature (Section 2.2). Cells with temperature higher than liquidus temperature are then converted from solid phase to liquid phase. Depending on the curvature of liquid–gas interface cells surface tension driven forces of wetting and capillarity set in. The phenomenon of wetting leads to the spreading of individual molten power particles on the underlying solid. For further details about the inclusion of wetting and capillarity effect the reader is directed to [25]. Effect of the surface tension is treated as a local modification of the gas pressure at the interface. It must be emphasized that the final meltpool does not assume a pre-defined geometrical shape based on analytical models. The collective effect of surface tension, capillary forces, Marangoni convection and recoil pressure (Section 2.2) are taken into account to calculate the dynamic meltpool shapes using LB method. The most important algorithms used in CALB model, e.g., for powder bed generation, simulation of fluid dynamics, heat transfer and grain solidification are presented next.

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