C. R. Mecanique ••• (••••) •••–•••

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Computational methods in welding and additive manufacturing/Simulation numérique des procédés de soudage et de fabrication additive

A two-dimensional simulation of grain structure growth within the substrate and the fusion zone during direct metal deposition

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ARTICLE INFO

Article history:
Received 24 January 2018
Accepted 11 April 2018
Available online xxxx

Keywords:
Finite element
Cellular automata
Grain morphology
Direct metal deposition
Decentered polygon algorithm

ABSTRACT

In this paper, a predictive multi-scale model based on a cellular automaton (CA)-finite element (FE) method has been developed to simulate thermal history and microstructure evolution during metal solidification for the Direct Metal Deposition (DMD) process. The macroscopic FE calculation that is validated by thermocouple experiment is developed to simulate the transient temperature field and cooling rate of single layer and multiple layers. In order to integrate the different scales, a CA–FE coupled model is developed to combine with thermal history and simulate grain growth. In the mesoscopic CA model, heterogeneous nucleation sites, grain growth orientation and rate, epitaxial growth, re-melting of pre-existing grains, metal addition, grain competitive growth, and columnar to equiaxed phenomena are simulated. The CA model is able to show the entrapment of neighboring cells and the relationship between undercooling and the grain growth rate. The model predicts the grain size, and the morphological evolution during the solidification phase of the deposition process. The developed "decentered polygon" growth algorithm is appropriate for the non-uniform temperature field. Finally, the single and multiple-layer DMD experiment is conducted to validate the characteristics of grain features in the simulation.

1. Introduction

Compared with the conventional subtractive manufacturing technologies, additive manufacturing (AM) has unique advantages including low heat input, small heat-affected zone, solid-free-form fabrication, near-net-shape, and so on. Direct Metal Deposition (DMD), a rapid developing AM technique, is able to manufacture a fully dense metal part without intermediate steps, which is especially appropriate for manufacturing heterogeneous components. During the deposition process, solidification thermodynamics determined by a series of process parameters affect microstructure evolution, which directly affects the mechanical properties of the materials. The temperature field history and the cooling rate are the key factor for controlling the solidification microstructure after the DMD process [1]. Several approaches, either stochastic or deterministic, have been taken to model solidification microstructure evolution. Anderson et al. [2,3] developed a Monte Carlo (MC) stochastic method to simulate the grain growth, topology, grain size distribution, curvature and grain velocities, as well as their interrelationships. Saito and Enomoto [4] incorporated the anisotropy of the grain boundary energy, the pinning effect

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https://doi.org/10.1016/j.crme.2018.08.003
1631-0721/

of precipitates on growth kinetics into the MC simulation. Another idea of modeling is the deterministic approach. Chen [5] investigated a phase-field (PF) method to model and predict mesoscale morphological and microstructure evolution in materials. Krill et al. [6–8] developed PF to simulate 2D grain growth, 3D gain growth, equiaxed solidification. However, a phase field model [9,10] usually carries a very high computational cost because of a requirement for a particularly fine computational grid.

In order to reduce the computational cost, RAPPAZ and GANDIN [11] put forward a two-dimensional cellular automaton approach to model grain structure formation in the solidification process. The model includes the mechanisms of heterogeneous nucleation and of grain growth. Nucleation occurring at the interface as well as in the liquid metal is treated by using two distributions of nucleation sites. The location and the crystallographic orientation of the grains are chosen randomly among a large number of cells and a certain number of orientation classes, respectively. However, the model was then applied to small Al–7wt%Si specimens of uniform temperature. In order to develop the non-uniform temperature prediction, Gandin et al. [12] proposed a 2-dimensional Cellular Automaton (CA) technique for the simulation of dendritic grain formation during solidification. The non-uniform temperature situation was fully coupled with an enthalpy-based Finite Element (FE) heat flow calculation. This progress made it possible to combine the temperature field history with the microstructure evolution. The coupled CA–FE model is applied to an Al–7wt%Si alloy. A three-dimensional CA–FE model predicting the dendritic grain structures formed during solidification [13] was analyzed. The potentiality of the CA–FE model is demonstrated through the prediction of typical grain structures formed during the investment casting and continuous casting processes. Based on the features of several developing approaches, Choudhury et al. [14] compared a CA model with a PF model for simulations of the dendritic solidification of an Al–4wt%Cu alloy, two- and three-dimensionally for different undercooling situations. In 2D, the tip properties simulated using the PF model show excellent agreement. At high undercooling, the CA model becomes advantageous, as its reproduction of the theoretical behavior improves. As the CA model is capable of simulating at coarse scales in a comparably short time, its output can be used as an input for a PF simulation for resolving finer details of microstructure formation. This can be utilized to build a hybrid model to integrate CA high efficiency and PF accuracy. Dore [15] investigated the quantitative prediction of micro-segregation during the solidification of the ternary alloy system, and applied it to the solidification of Al–Mg–Si. Jarvis et al. [16] firstly compared 1D, 2D, and 3D cellular automaton finite difference (CA–FD) simulations of the non-equilibrium solidification in an Al–3.95Cu–0.8Mg ternary alloy. It has been demonstrated that there is good agreement between all CA–FD models in terms of primary α-Al phase. However, the final dendrite arm spacings are slightly overestimated in 2D and 3D.

High cooling rate and non-equilibrium is a typical characteristic of the DMD technique comparing the conventional casting process and simulation. Grujicic et al. [17] proposed a modified CA-based method to investigate the evolution of the solidification grain microstructure during the LENS rapid fabrication process. This research established the relationship between process parameters (e.g., laser power, laser velocity) and solidification microstructure in binary metallic alloys. The finite difference analysis was also coupled with the modified CA to calculate the temperature field as the input of microstructure prediction. Kelly et al. [18,19] developed the thermal history in DMD of Ti6Al4V and microstructural characterization. Tan et al. [20] developed a multi-scale model to study the growth of grains and sub-grain dendrites of austenitic stainless steel during laser keyhole welding process. Chen et al. [21,22] developed a 3D coupled CA–FE model for the solidification grain structure during Gas Tungsten Arc Welding (GTAW). During the simulation, the parallel computations and dynamic strategies for the allocation of CA grids are employed to optimize the computer memories. It provides the possibility of handling domains with millions of grains inside. Zinoviev et al. [23] investigated a two-dimensional numerical model to simulate the grain structure evolution during a selective laser melting process. The equiaxed and columnar grains, which is validated by the experimental result, can be achieved within the melt pool. However, there are few investigations on microstructure evolution prediction based on the whole deposit part during the DMD process. This part-level simulation on microstructure is critical because it provides the foundation for predicting and controlling the mechanical properties.

In this study, a predictive multi-scale model based on a Cellular Automaton (CA)-Finite Element (FE) method has been developed to simulate the thermal history and microstructure evolution during metal solidification in the frame of a laser-based additive manufacturing process. ABAQUS was used to calculate the temperature field of the whole part, which offers the macroscopic FE nodes' temperature. In order to integrate the different scales, a coupled model is developed to combine with thermal history and simulate nucleation site, grain growth orientation and rate, epitaxial growth of new grains, remelting of preexisting grains, metal addition, and grain competitive growth. Interpolation was utilized to obtain the finer nodes' temperature based on the FE nodes result. The temperature field was validated by type-K thermocouples. The CA model, which was able to show the entrapment of the neighboring cells and the relationship between undercooling and grain growth rate, was built to simulate microstructure information, such as grain size and columnar grain orientation. The developed "decentered polygon" algorithm is more appropriate for grain structure development in the highly non-uniform temperature field. This simulation will lead to new knowledge that simulates the grain structure development of single-layer and multiple-layer deposition during the DMD process. The microstructure simulation results were validated by the experiment. The model parameters for the simulations were based on a Ti–6Al–4V material (Fig. 1).

Please cite this article in press as: J. Zhang et al., A two-dimensional simulation of grain structure growth within the substrate and the fusion zone during direct metal deposition, C. R. Mecanique (2018), https://doi.org/10.1016/j.crme.2018.08.003