



Dendrite growth simulation during solidification in the LENS process

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Abstract

A two-dimensional model combining the finite element method and the cellular automaton technique was developed to simulate dendritic growth occurring in the molten pool during the laser-engineered net shaping (LENS) process. Based on the simulation results and previously published experimental data, empirical expressions describing the relationship between the cooling rate and the dendrite arm spacing (DAS) were proposed. In addition, the influence of LENS process parameters, such as the moving speed of the laser beam, the layer thickness and the substrate size, on the DAS was also discussed. Finally, different dendrite morphologies calculated at different locations were explained based on local solidification conditions. The simulation results showed good agreement with previously published experiments. This work contributes to the understanding of microstructure formation and the resulting mechanical properties of LENS-built parts as well as providing a fundamental basis for optimization of the LENS process.

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1. Introduction

Laser-engineered net shaping (LENS) is a rapid fabrication process developed by Sandia National Laboratories in the late 1990s. Owing to its cost-saving potential and the fine microstructure resulting from the high cooling rate, it is gaining popularity as a rapid prototyping and repairing technology [1–3]. Many samples have been tested to prove the good mechanical properties obtained by LENS, such as yield strength, ultimate strength and hardness for various kinds of steels (SS304 [4,5], 308 [6], 316 [7], AISI4140 [8], H13 [9,10]) and other alloys (Ni alloy [11], Ti alloy [11,12], Cu alloy [7], Al alloy [12]). Some comparisons [5,7,11] were made between the deposition materials obtained by LENS and those obtained by other processing methods, and the results showed that the LENS parts have better mechanical properties owing to the very fine microstructure produced by the high cooling rate.

Kurz [13], Kelly and Kampe [14] and Colaco and Vilar [15] proposed that the microstructure and mechanical properties of the LENS components depend partly on the solid-state transformation while cooling to room temperature. However, the transformations are driven mainly by the consecutive thermal cycles when the laser beam moves along the deposited surface layer by layer. Hence, much work has been done to characterize the thermal behavior during the LENS process by conducting experiments [16–20] and developing mathematical models [21–26]. Hofmeister et al. [17] employed a digital video camera with thermal imaging techniques to observe the molten pool and analyze the temperature gradients and cooling rates in the vicinity of the pool region. Griffith et al. [20] inserted a fine diameter (10 μm) type C thermocouple directly into the sample to obtain the *in situ* thermal history data during LENS fabrication. Many mathematical models, both two-dimensional (2D) [21–24] and three-dimensional (3D) [25,26], have also been developed to try to establish an understanding of the thermal behavior in the LENS process by the finite element (FE) or finite difference method. That research on the thermal behavior

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during the LENS process helped to improve understanding of the microstructure formation.

The microstructure, which is determined by the thermal history and also controls the mechanical properties, gained more and more attention, and many experiments have been done to analyze the microstructure, especially the grain size (dendrite arm spacing (DAS) for columnar dendrite) and morphology. Experiment results have proved that very fine microstructures are formed as a result of the high cooling rates and temperature gradients. Ghosh and Choi [27] deduced an equation which describes the relationship between the DAS and the thermal behaviors and, based on the equation, the DAS was calculated to evaluate the microstructure. Very few papers [21,28] have been published on the numerical modeling of the microstructure evolution during solidification and solid-state phase transformation while cooling to room temperature, with scarce or no details on the dendrite morphology and growth process.

This paper focuses on the microstructural evolution of the solidification process: DAS and dendrite morphology and the influence of LENS process parameters on the solidification. Deterministic (phase-field (PF)) and stochastic (cellular automaton (CA)) methods are usually applied to simulate dendrite growth during solidification. The PF method [29–31] simulates the phase types by solving governing differential equations which describe the evolution of phase field variables for either pure metals or multi-component alloys. The CA technique can simulate the dendrite morphology by determining the solid/liquid interface based on temperature and solute fields. This method needs fewer computer resources than PF, although artificial anisotropy can be introduced by the CA mesh. Rappaz and Gandin [32,33] initially coupled the CA and FE methods to obtain the thermal field and the grain structure of an Al–Si alloy. Sanchez and Stefanescu [34], Zhu and Hong [35] and Zhu and Stefanescu [36] proposed a dendrite growth CA model by tracking the interface based on the virtual front tracking method for Al–Cu and Fe–C alloys. Dong and Lee [37] used the CA–finite difference method to simulate the columnar-to-equiaxed transition during the directional solidification of an Al–Cu alloy. 3D models [38,39] were also used, which combine the CA and FE methods to simulate the dendrite growth in binary alloys controlled by solute diffusion. Most of these fundamental works on microstructure evolution did not solve the energy equation, but were based on a prescribed temperature field (constant cooling rate was used to simulate the temperature field). In Ref. [40], a FE–CA scheme was applied to simulate the dendrite growth in a laser welding pool, but the calculated DAS was $\sim 100\text{ }\mu\text{m}$, which is much larger than the DAS expected in LENS microstructures. In the present work, a new FE–CA technique is developed which is able to capture the evolution of the fine microstructure occurring during solidification in a LENS pool.

2. Background

2.1. Columnar grain formation in LENS

Different dendrite morphologies can be obtained by controlling the thermal gradient and cooling rates (solidification velocity) in the molten pool [41–43]. Bontha et al. [44] determined the relationship between the dendrite morphology, the temperature gradient (G) and solidification velocity (R) during the LENS process by plotting points in G vs. R space. The authors found that the resulting grain morphology can be predicted as columnar, equiaxed or mixed. The conditions of laser power and laser travel speed for a fully columnar dendritic structure are also obtained in LENS-deposited Ti–6Al–4V thin walls.

The microstructure in the deposited part is very complicated because it undergoes a near rapid solidification process and several solid-state phase transformations during cooling to room temperature. Owing to the lack of recrystallization of the last layer in the multi-layer deposition of the LENS process, the microstructure of the last layer differs from that of the other layers. Cellular and dendritic structures have been observed in the deposition layers [45–48]. A dendritic structure was usually found in last layer, while a dendrite/cell structure was found in the previous layers [49–55]. Columnar dendrites were observed in the last layer in SS316L [54]. The cell structure of SS316 after cooling to room temperature was also obtained [55]. A dendritic microstructure can also occur in layers other than the last one. The top layer showed a mainly dendritic structure, and this structure was also observed at layer boundaries [50]. It can be identified that the microstructure of the last layer differs from others partly because all the other layers were tempered during deposition of the next layer except for the last one. All the above reports provide clear evidence that dendritic structures can occur during solidification in the LENS process.

2.2. DAS and cooling rate

Solidification microstructure and grain size influence the recrystallization process and hence the mechanical properties of LENS parts. The DAS, which is influenced significantly by cooling rate, is often used to evaluate the solidification microstructure. Several experiments have been conducted to study the relationship between the cooling rate ε (K s^{-1}) and DAS λ , and these showed that a linear relationship exists between $\log \lambda$ and $\log \varepsilon$ [56]. A general relationship between ε and secondary DAS (SDAS) (λ_2 , in μm) was experimentally determined as $\lambda_2 = 25\varepsilon^{-0.28}$ for 310 stainless steel in laser welding [57].

In the present paper, a 2D FE method coupled with a CA technique is developed to calculate the dendritic growth during solidification in the molten pool during LENS deposition of a single layer of Fe–0.13 wt.% C. The model solves the conservation equations of heat and mass transfer in order to calculate the temperature field,

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