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ScienceDirect

Acta Materialia 69 (2014) 47–59

Acta MATERIALIA

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Simulation of diffusion-limited lateral growth of dendrites during solidification via liquid metal cooling

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Received 3 September 2013; received in revised form 16 January 2014; accepted 17 January 2014
Available online 23 February 2014

Abstract

Directional solidification via the liquid metal cooling process results in refined microstructure and reduced defects, thus providing improved mechanical performance of single crystal (SX) materials. However, the enhanced heat extraction inherent to the process results in a curved solidification front that may lead to non-axial growth of dendrites near the casting walls. The mechanism by which the lateral growth occurs has been investigated by microstructure modeling via solute-adjusted, diffusional growth of dendrites. Local thermal profiles derived from continuum solidification models were used as inputs to a dendrite-growth model capable of simulations in both two and three dimensions. A finite difference calculation of the diffusion field and volume of fluid tracking for the growth of the dendrite front was coupled to predict the microstructure evolution during directional solidification. Model predictions were compared to experimentally observed dendritic structures. In addition, a parametric analysis was conducted to evaluate the sensitivity of the dendrite-growth mode to changes in thermal, structural (such as dendrite position and spacing) and model parameters. The inclination angle of the solidification front strongly influenced the evolution of dendritic structure. The degree of misorientation of the $\langle 001 \rangle$ SX orientation from the withdrawal axis significantly contributed to the onset of lateral dendritic growth.
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Keywords: LMC directional solidification; Microstructure modeling; Dendrite growth

1. Introduction

The liquid metal cooling (LMC) process is based on the concept of the Bridgman process for directional solidification [1] but utilizes a liquid–metal coolant to extract heat from the mold more efficiently [2–8]. The benefits of the process have been identified, especially for large cross-section components requiring significant heat extraction to maintain directional solidification [3–15]. Despite the benefits of the process, the potential for a curved solidification front and change in dendrite morphology is increased [4,5].

One possible consequence of a curved solidification interface is lateral growth, the overgrowth of well-aligned primary dendrite arms by secondary arms of neighboring dendrites growing transverse to the withdrawal direction (Fig. 1) [5]. Lateral growth is a precursor to nucleation of misoriented grains, which are detrimental to single-crystal components [5]. In addition, an increased propensity for defect formation has been identified in the boundary between regions of axial growth and lateral growth within the dendrite structure due to the competition between two

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http://dx.doi.org/10.1016/j.actamat.2014.01.035
1359-6454/Published by Elsevier Ltd. on behalf of Acta Materialia Inc.

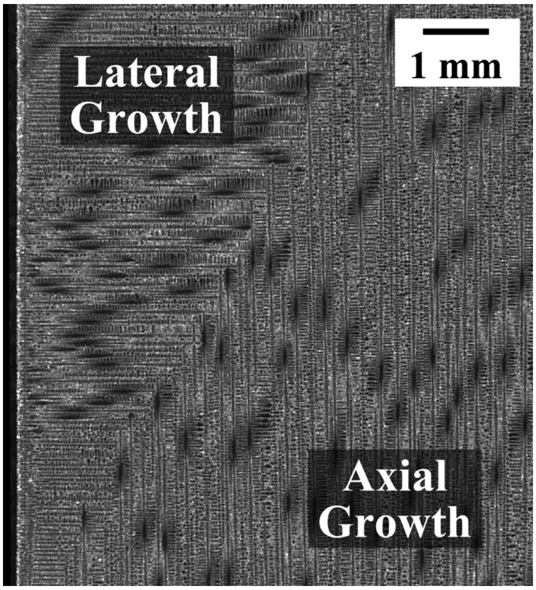

Fig. 1. Longitudinal micrograph of lateral growth. Note that the withdrawal direction is vertical and the surface of the casting is on the left side of the image [5].

colliding growth fronts [6]. Further understanding of the mechanism for the onset of lateral growth is needed as related to local thermal conditions, independent of mold geometry.

The morphological evolution of dendrites under axial growth conditions has been modeled extensively over the past few decades. Dendrite growth models utilizing phase field [16,17], dendrite grain envelope [18,19], level set [20–25], combined finite difference (FD) with either cellular automata or volume of fluid [26–36], geometric [37] or front-tracking [38] techniques have been developed. One weakness of these modeling approaches is the limitation of model size and time scale, due to their computational expense [39]. Additionally, the ability to directly validate the dendrite-growth predictions via experiments limits their widespread acceptance. Investigation of multi-component engineering alloys is a further challenge due to the order-of-magnitude increase in computation time in ternary and higher-order systems and the difficulty of obtaining the corresponding alloy properties.

Experiments utilizing a transparent polymer analog were conducted to study the evolution of dendritic structure [40–50]. Grugel and Zhou considered off-axis heat flow relative to the dendrite-growth direction and identified changes in primary dendrite arm spacing with off-axis heat flow. They observed the onset of lateral growth at a solidification-front inclination angle of 45° [40]. Other efforts also evaluated off-axis growth of dendrites through utilization of the polymer analog [41]. While these experiments were valuable with respect to understanding the mechanisms of dendrite growth, the thermal environment in which they were conducted was not directly representative of an investment casting environment typically employed for the growth of single crystals (SXs).

Likewise, modeling the evolution of dendritic growth at the scale of the dendritic structure in the presence of thermal conditions representative of the investment casting environment is also less common than the uniformly imposed thermal conditions representative of a laboratory environment [9]. The validation of model predictions of dendrite growth with experimental measurement under processing-representative conditions is rare [9,11]. Simulation of the thermal characteristics of the LMC process at the continuum scale has demonstrated the value of modeling in conjunction with careful experimentation [4,5,11,12,51]. However, no dendrite-scale modeling has yet been conducted with a consideration of the unique thermal characteristics of the LMC process.

Recently reported experiments [5] highlight the importance of the solidification-front inclination angle at the surface of the mold. Lateral growth and the presence of nucleated grains were predicted with consideration of the thermal field at the component scale during the LMC solidification process. However, the evolution of dendritic structure is controlled by the local thermal condition and solute diffusion at the solid–liquid interface [39]. Thus, there is a need to consider the thermosolutal kinetics of directional solidification at the scale of the dendrite structure under complex thermal conditions that depart from the ideal model of axial heat extraction during directional solidification. This information could provide key insights into the mechanisms associated with transitions in the mode of dendritic growth and instabilities that lead to the breakdown of the directional solidification process. Based on the understanding at the microstructure scale, macroscopic criteria functions for the component scale could be enhanced by a better understanding of the underlying mechanisms. With utilization of the LMC process, there may be a need for new defect-formation criteria to aid identifying preferred process conditions and the prediction of dendritic scale.

In this research, thermal conditions from continuum solidification models [5] are used as inputs to a microstructure model that predicts dendrite structure from solute diffusion and the thermal field. Due to the accompanying experimental observations previously reported, the evaluation of a model that incorporates continuum-scale thermal predictions with the meso-scale evolution of solute and dendrite structure is possible. Conditions under which lateral growth occurs are identified. Fundamental insights into the mechanism of lateral growth are enhanced via a comprehensive series of parametric analyses that consider alloy properties, dendrite packing, crystal orientation and local process variations in both two and three dimensions.

2. Modeling methods

The modeling approach consists of a FD calculation of the diffusion field and a volume-of-fluid type tracking of the change in solid fraction, which advances the propagation of dendrites together with a modified