Original Research

# Multi-scale simulation of single crystal hollow turbine blade manufactured by liquid metal cooling process 

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#### Abstract

Liquid metal cooling (LMC) process as a powerful directional solidification (DS) technique is prospectively used to manufacture single crystal (SC) turbine blades. An understanding of the temperature distribution and microstructure evolution in LMC process is required in order to improve the properties of the blades. For this reason, a multi-scale model coupling with the temperature field, grain growth and solute diffusion was established. The temperature distribution and mushy zone evolution of the hollow blade was simulated and discussed. According to the simulation results, the mushy zone might be convex and ahead of the ceramic beads at a lower withdrawal rate, while it will be concave and laggard at a higher withdrawal rate, and a uniform and horizontal mushy zone will be formed at a medium withdrawal rate. Grain growth of the blade at different withdrawal rates was also investigated. Single crystal structures were all selected out at three different withdrawal rates. Moreover, mis-orientation of the grains at $8 \mathrm{~mm} / \mathrm{min}$ reached $\sim 30^{\circ}$, while it was $\sim 5^{\circ}$ and $\sim 15^{\circ}$ at $10 \mathrm{~mm} / \mathrm{min}$ and $12 \mathrm{~mm} / \mathrm{min}$, respectively. The model for predicting dendritic morphology was verified by corresponding experiment. Large scale for 2D dendritic distribution in the whole sections was investigated by experiment and simulation, and they presented a well agreement with each other.


## 1. Introduction

Turbine blades as a key component in turbine engines play the most important role in the modern advanced aviation and energy industry [1-3]. Nickel-based superalloys are widely used in manufacturing the turbine blades, because of their high temperature fatigue resistance, creep strength, and corrosion resistance [4-6]. Single crystal (SC) turbine blades exhibit even better comprehensive performance due to the elimination of grain boundary and strictly control the crystallographic orientation [7-10]. As we know, directional solidification (DS) process has significantly promoted the development of SC superalloy castings over the past few decades [11-13]. The most common DS technique is Bridgman process, i.e. high-rate solidification (HRS) process in the current naming rules [14]. However, some issues occurred frequently due to the fact that it provide poor ability of heat transfer and the lower temperature gradient in HRS process, such as warping and crack of shell mold, ceramic-metal reaction, and low-yield of shell mold at high temperature, and freckles, stray grains were formed in the castings [15-17]. All of these problems originate from the low rate of heat
transfer of HRS process. Therefore, several possible techniques were being evaluated for improve the heat transfer efficiency and the temperature gradient, which include liquid metal cooling (LMC) process [18,19], fluidized-bed quenching (FBQ) process [20], and gas cooling casting (GCC) process [21]. Among of these techniques, LMC process has the longest development history which improves the heat transfer by immersing the molten metal and the ceramic mold into a container with low melting temperature liquid metal coolant as they are withdrawn from the heating zone [22]. The schematic of LMC process is shown in Fig. 1. Liquid metal coolant is stannum, and many small ceramic beads float on the surface of the liquid stannum as a conforming thermal barrier between the heating and cooling zones of the furnace. When the ceramic mold was withdrawn in liquid stannum, the heat transfer pattern changed to convection heat on the mold surface, and convection heat transfer is more efficient than radiation heat transfer. Therefore, the withdrawal rate can reach as fast as $30 \mathrm{~mm} \min ^{-1}$ for the production of castings while maintaining higher temperature gradient by using LMC process [23], and this potential capability of faster withdrawal rate can reduce porosity defects of

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Fig. 1. Schematic illustration of LMC furnace.
castings [24]. In addition, LMC process can also reduce the primary dendrite arm spacing (PDAS), and refine $\gamma^{\prime}$ and carbide morphologies [25]. However, to date, the LMC process is still in experimental stage due to the parameters are unmanageable, and it will be a long time before put into production.

Since microstructures are the strategic link between process and performance, an understanding of microstructure evolution is required in order to improve the properties of the blades. In recent few years, computational capability for evaluating the microstructure evolution during LMC process has been developed [26]. Elliott et al. [27] investigated the influence of withdrawal rate on the mushy zone shape and microstructure morphology during LMC process, and the results showed that an excessive withdrawal rate will result in a concave interface of the mushy zone and the microstructure growing preferentially toward the center; whereas, mushy zone presented a convex interface and microstructure grew dispersedly at a smaller withdrawal rate. Kermanpur et al. [28] simulated the grain structure evolution of an industrial gas turbine blade prepared by LMC process using a cellular automaton (CA) coupled with finite element (FE) model inside the commercial software ProCAST. CA method is a powerful computational approach that can reveal a wide range of micro or meso scale structure features, which was developed by Rappaz and Gandin [29-31] in the 1990s. Subsequently, researchers focused their attentions on the simulation of dendrite growth and their evolution behavior using CA model. Wang et al. [32] developed the cellular automaton-finite difference (CA-FD) model considered the solute diffusion to simulate dendrite growth of binary alloys, and found that perturbations significantly reduced the range of stable primary dendrite spacing. Miller et al. [33] investigated the LMC process of castings through microstructure simulation, and proposed a lateral growth model for dendrite growth. The model indicated that the enhanced heat extraction inherent to the process resulted in a curved solidification front that may lead to a non-axial dendrite growth near the casting walls. Recently, Zhang et al. [34] simulated the directional dendrite growth behavior and morphology based on CA-FD model, and the model was coupled with the macro DS parameters such as withdrawal rate and pouring temperature. However, the simulation studies were just confined to 2D or pseudo 3D scales due to the limitation of computational capability. Although some techniques such as the parallel computing and adaptive mesh refinement methods have been developed in order to enhance computational efficiency, multi-scale simulation of microstructure
evolution in a whole blade is still a challenge.
The aim of this paper is to build a multi-scale model coupling with the energy conservation, nucleation and growth and solute diffusion in order to simulate the macro temperature field distribution, meso grain growth and micro dendritic morphologies of the blade during LMC process. The mushy zone evolution will be analyzed based on simulation results of temperature field. Grain structures of the blade at different withdrawal rates are also predicted, and the mis-orientation of these grains will be discussed in detail. The model for predicting dendritic morphology in the blade will be verified by corresponding experiment, and large scale for 2D dendritic distribution over the entire sections of blade are investigated by experiment and simulation.

## 2. Models description and experimental procedure

### 2.1. Temperature field model

Heat transfer condition is complex in LMC process, so an integrated boundary condition was established to simulate the temperature fields. The basic physical process can be described based on law of the conservation of energy, and the energy conservation equation [11] is described as follows:
$\rho c_{\mathrm{p}} \frac{\partial T}{\partial t}=\lambda \cdot \nabla^{2} T+\rho \Delta H \frac{\partial f_{\mathrm{s}}}{\partial t}+Q_{\mathrm{net}}$
where $T$ is the temperature, $t$ is the time, $\rho$ is the density, $c_{\mathrm{p}}$ is the specific heat, $\Delta H$ is the latent heat, $\lambda$ is the heat conductivity, $f_{\mathrm{s}}$ is the mass fraction of solid phase, and $Q_{\text {net }}$ is the heat flux between the solid elements. A modified Monte Carlo-based ray tracing model [24] was adopted to deal with the heat radiation between every two discrete surfaces. However, when the heat transfer pattern varied from radiation to conduction as the shell mold was descended into the cooling zone, and the heat flux, $Q_{\text {net }}$, will be treated as heat conduction, which described as follows:
$\left\{\begin{array}{cc}Q_{\text {net }}=\sigma \sum_{n=1}^{N} \frac{\beta_{n}\left(T^{4}-T_{n}^{4}\right)}{\frac{1-\varepsilon}{\varepsilon}+\frac{\left(1-\varepsilon_{n}\right) S}{\varepsilon_{n} S_{n}}+1} & z>h+h_{b} \\ Q_{\text {net }}=\alpha_{b}\left(T-T_{a}\right) & \mathrm{h}<z \leq h+h_{b} \\ Q_{\text {net }}=\alpha\left(T-T_{a}\right) & z \leq h\end{array}\right.$
where $\sigma$ is the Stefan-Boltzmann constant, and the value equals $5.67 \times$ $10^{-8} \mathrm{~W} \cdot \mathrm{~m}^{2} \cdot \mathrm{~K}^{-4}, N$ is the numbers of ray lines, $\beta_{\mathrm{n}}$ is the energy factor of $n, T, T_{\mathrm{a}}$ and $T_{\mathrm{n}}$ are the temperature of different solid elements, $\varepsilon$ is the blackness coefficient, $S$ and $S_{\mathrm{n}}$ are the surface area of different elements, $\alpha$ and $\alpha_{\mathrm{b}}$ are the heat transfer coefficient of different boundaries, $h$ is liquid level of the liquid metal coolant, and $h_{\mathrm{b}}$ is the thickness of the ceramic beads (Fig. 1).

### 2.2. Grain structure model

The grain structure simulation is based on the modified CA method [35]. A stochastic nucleation model was established to calculate the nucleus number as follows:
$\frac{\partial N}{\partial(\Delta T)}=\frac{N_{S}}{\sqrt{2 \pi} \Delta T_{\sigma}} \exp \left[-\frac{\left(\Delta T-\Delta T_{N}\right)^{2}}{2\left(\Delta T_{\sigma}\right)^{2}}\right]$
where $N$ is the nucleus density, $\Delta T$ is the undercooling, $N_{\mathrm{s}}$ is the maximum nucleus density, $\Delta T_{\sigma}$ is the standard deviation of the distribution, and $\Delta T_{\mathrm{N}}$ is the average nucleation undercooling. Then the grain density can be described as follows:
$N(\Delta T)=\int_{0}^{\Delta T} \frac{d N}{d\left(\Delta T^{\prime}\right)} d\left(\Delta T^{\prime}\right)$
where the $\Delta T^{\prime}$ is the integral unit of undercooling.
The grain growth is calculated based on the KGT equation [36], and the growth rate at the grain tip, $v(\Delta T)$, can be described as follows:

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