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Multi-scale simulation of directional dendrites growth in superalloys

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ABSTRACT

The directional dendrite growth behavior and morphology were simulated based on the cellular automaton-finite difference (CA-FD) considering macro directional solidification (DS) parameters such as withdrawal rate and pouring temperature. Two types of directional dendrite growth models were proposed to realize the multi-scale simulation. A 3D dendrite growth model based on heat transfer and solute diffusion was built to simulate the dendrite growth during a real DS process, which is proved useful for the detail dendrite growth and morphology prediction at a micro 3D scale. A modified shaped function model was proposed to predict the evolution behavior of a large number of dendrites in the entire section of a DS cast sample at a macro scale, based on which the evolution behavior of thousands of dendrites was predicted in the 2D section during the DS process. In these models, the temperature interpolation algorithm and the dendrite orientation mathematical projection were used to transfer information between macro DS process calculation and micro dendrite growth simulation. The corresponding DS experiment was performed to verify the numerical models, and they agreed well. The DS dendritic evolution behavior and detail morphology, especially thousands of dendrites distribution at a large scale, were successfully simulated based on the two models proposed on the condition of a real DS process.

1. Introduction

The high-performance turbine blades used in modern advanced aero and power industry engines are produced by the DS process and made up of directional columnar grains or single crystal structure. DS dendrite as substructure of the directional columnar grains or single crystal highly influences the final serving property of these blades. Trivedi and Kurz (1994) had systematically summarized the important aspects of dendrite growth and earlier theories, including the dendritic growth model in the DS process. Subsequently, there have been several studies on the simulation of DS dendrite growth and their evolution behavior using various numerical methods. Among these methods, phase field (PF) and cellular automaton (CA) developed rapidly and widely used. The PF model primarily includes factors such as the surface energy of the crystal, kinetics of the dendritic tip, and grain preferential orientation. This method is useful for describing the detailed morphology of a dendrite in two and even three dimensions (Karma and Rappel, 1998). However, only the growth of several dendrites could be predicted because of the need for enormous calculations.

CA is another powerful method for predicting dendrite growth. It integrates deterministic modeling and stochastic modeling and shows great advantages in grain structure simulation over a large scale. Nastac (1999) had simulated solidification morphologies and segregation patterns in cast dendritic alloys over 10^{-4} m using such as a uniform temperature field distribution as boundary condition, Pan and Zhu (2010) built a modified CA model for dendritic growth which is good for simulating the details of the dendrite morphology. However, these models barely considered the macro solidification parameters, which implies that some boundary and initial conditions need to be assumed. Pan et al. (2010) predicted grain competitive growth of a single crystal selection process at the 10^{-1} m scale, which considered macro solidification parameters such as pouring temperature, cooling speed, and withdrawal rate but without simulation of dendrite growth.

It is well known that the key problem of predicting dendrite growth in the macro scale is the amount of calculation required. Even though parallel computing technologies have been proposed to solve the calculation problem, it is still difficult to model the growth of a huge number of dendrites over a large scale. For example, Shimokawabe et al. (2011) predicted the growth of a few

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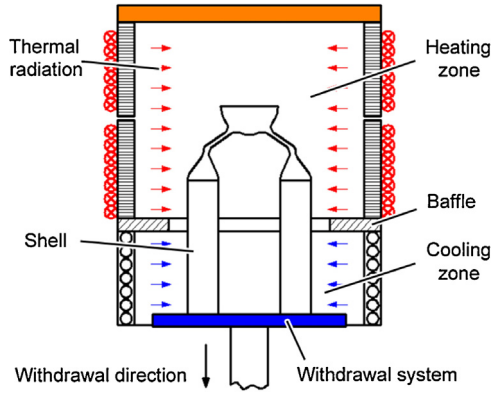

Fig. 1. Schematic of Bridgman furnace.

dendrites over the micrometer scale on the SUBAME 2.0 supercomputer. However, the real solidification process always includes thousands of dendrites growing competitively in the macro scale.

In this study, a 3D model and a modified shaped function model for dendrite growth are proposed to simulate dendrite growth during a real high rapid solidification (HRS) process in the macro scale. Here, HRS was the main method used in the DS casting. The equipment used in the HRS method is the Bridgman furnace, shown in Fig. 1. In a real HRS process, there are two ways of heat dissipation: heat conduction and heat radiation. The heat radiated from the sides leads to inclined, concave, or convex isothermal surfaces directly, which are quite different from ideal horizontal isothermal surfaces. As for the HRS process, the dendrite growth behavior will be complicated and different from the ideal assumption of homogeneous temperature gradients, which was reported in a previous study (Zhang et al., 2011). In the present study, solidification parameters such as withdrawal rate and pouring temperature were considered during the simulation calculation. The 3D DS superalloy dendritic morphology in the target local domain and 2D whole-section dendritic distribution were simulated. The simulated results were verified using experimental results, and both were in good agreement.

2. Mathematical models and experimental methods

2.1. The 3D dendrite growth model

The DS dendrite growth was influenced by solute distribution and temperature field. The solute distribution directly affects the dendrite morphology and dendrite arm spacing. In the 3D dendrite growth model, the solute distribution was calculated and was coupled with the temperature field calculation. The solute diffusion was governed by Eq. (1) in the bulk of the liquid and the solid phase.

$$\frac{\partial C_i}{\partial t} = D_i \left(\frac{\partial^2 C_i}{\partial x^2} + \frac{\partial^2 C_i}{\partial y^2} + \frac{\partial^2 C_i}{\partial z^2} \right) i = L, S \tag{1}$$

At the interface of the liquid and solid, solute diffusion was controlled by Eq. (2).

$$C_S^* = k_e C_L^* \tag{2}$$

In this equation, C_S^* is the solute in the solid at the liquid/solid interface, C_L^* is the solute in the liquid at the liquid/solid interface, and k_e is the solute partition coefficient.

The solute conservation equation (Nastac, 1999) is described as follows:

$$v_n C_L^* (1 - k_e) = D_L \left(\frac{\partial C_L}{\partial x} + \frac{\partial C_L}{\partial y} + \frac{\partial C_L}{\partial z} \right) - D_S \left(\frac{\partial C_S}{\partial x} + \frac{\partial C_S}{\partial y} + \frac{\partial C_S}{\partial z} \right) \tag{3}$$

Then, the growth velocity (v_n) of the dendrite can be obtained. C_L^* could be calculated using Eq. (4) (Nastac, 1999).

$$C_L^* = C_0 + \frac{1}{m_L} \cdot \left[T^* - T_{Liq} + \Gamma \kappa f\left(\theta_i\right) \right] \tag{4}$$

In this equation, C_0 is the original solute concentration in the liquid, T^* is the temperature at the liquid/solid interface, $T^* - T_{Liq}$ is the undercooling caused by heat dissipation, T_{Liq} is the temperature of the liquidus, $\Gamma \kappa f\left(\theta_i\right)$ is the undercooling caused by the curvature, Γ is the Gibbs-Thomson coefficient, κ is the curvature of the liquid/solid interface, and $f\left(\theta_i\right)$ is the anisotropy function at the liquid/solid interface.

$$\kappa = \frac{1}{a_m} \left[1 - \frac{2}{125} \sum_{i=1}^{125} f_S(i) \right] \tag{5}$$

$$f\left(\theta_i\right) = \prod_{i=l,m,n} [1 + \gamma \cos(K_i \theta_i)] \tag{6}$$

In the above equations, $f_S(i)$ is the solid fraction of the i cell, a_m is the micro grid step length, γ is the anisotropy strength coefficient, K_i is the anisotropic modulus, and θ_i is the interface anisotropy angle, and l, m, and n are the coordinates.

2.2. The modified shaped function model

The 3D simulation of dendrite growth for the entire DS cast sample is difficult because of the large amount of calculations and the enormous memory usage. In this study, the 3D dendritic growth model was simplified by a proposed modified shaped function to reduce the calculation amount greatly, and then, dendrite growth could be predicted in the entire cross section of a DS cast sample.

The shaped function method was once used to simulate grain growth (Xu et al., 2002), which is controlled by a simple equation as follows:

$$L(\theta) = L_0[1 + (A - 1)\cos 4\theta] \tag{7}$$

In this equation, $L(\theta)$ is the polar radius in polar coordinates, L_0 is the initial length of the polar radius, A is the shape factor that decides the profile of the figure described, and θ is the polar angle.

The equation for 2D axis transformation regarding the growth orientation of the second dendritic arm is described using Eq. (8).

$$\begin{cases} x' = (x - x_0)\cos\theta + (y - y_0)\sin\theta \\ y' = (y - y_0)\cos\theta - (x - x_0)\sin\theta \end{cases} \tag{8}$$

In Eq. (8), x' and y' are the coordinates in the $x'oy'$ system, which is a rotated Cartesian coordinate system of the xoy system, x_0 and y_0 are the symmetric center coordinates in the $x'oy'$ system, and θ is the rotated angle of the secondary dendritic arms.

Based on the 3D transformation equation, the dendritic morphology in the transverse section could be calculated at the Euler angles (ϕ_1, ψ, ϕ_2) of different dendrites. The modified shaped function is shown in Eq. (9) in a certain section of the DS sample, and the specific derivation process is shown in the Appendix A.

$$\begin{aligned} x' &= A_1 x + A_2 y + A_3 z_0 + x_0 \\ y' &= B_1 x + B_2 y + B_3 z_0 + y_0 \end{aligned} \tag{9}$$

where

$$A_1 = \cos\phi_1 \cos\psi \cos\phi_2 - \sin\phi_1 \sin\phi_2 + \cos\phi_1 \sin\psi \tan\psi \cos\phi_2$$

$$A_2 = \sin\phi_1 \cos\psi \cos\phi_2 - \cos\phi_1 \sin\phi_2 + \sin\phi_1 \sin\psi \tan\psi \cos\phi_2$$

$$A_3 = \sin\psi \cos\phi_2 \cos\psi^{-1}$$