Journal of Crystal Growth 479 (2017) 22–33

Contents lists available at ScienceDirect

Journal of Crystal Growth

journal homepage: www.elsevier.com/locate/crys

Numerical simulation of dendrite growth in nickel-based superalloy and validated by in-situ observation using high temperature confocal laser scanning microscopy

Xuewei Yan, Qingyan Xu *, Baicheng Liu

Key Laboratory for Advanced Materials Processing Technology, Ministry of Education, School of Materials Science and Engineering, Tsinghua University, Beijing 100084, China

ARTICLE INFO

Article history:
Received 10 June 2017
Received in revised form 19 September 2017
Accepted 20 September 2017
Available online 21 September 2017
Communicated by T.F. Kuech

Keywords:
Numerical simulation
Dendrite growth
In-situ observation
HT-CLSM

ABSTRACT

Dendritic structures are the predominant microstructural constituents of nickel-based superalloys, an understanding of the dendrite growth is required in order to obtain the desirable microstructure and improve the performance of castings. For this reason, numerical simulation method and an in-situ observation technology by employing high temperature confocal laser scanning microscopy (HT-CLSM) were used to investigate dendrite growth during solidification process. A combined cellular automaton-finite difference (CA-FD) model allowing for the prediction of dendrite growth of binary alloys was developed. The algorithm of cells capture was modified, and a deterministic cellular automaton (DCA) model was proposed to describe neighborhood tracking. The dendrite and detail morphology, especially hundreds of dendrites distribution at a large scale and three-dimensional (3-D) polycrystalline growth, were successfully simulated based on this model. The dendritic morphologies of samples before and after HT-CLSM were both observed by optical microscope (OM) and scanning electron microscope (SEM). The experimental observations presented a reasonable agreement with the simulation results. It was also found that primary or secondary dendrite arm spacing, and segregation pattern were significantly influenced by dendrite growth. Furthermore, the directional solidification (DS) dendritic evolution behavior and detail morphology were also simulated based on the proposed model, and the simulation results also agree well with experimental results.

1. Introduction

Nickel-based single crystal (SC) superalloys are widely used in modern advanced aero and power industry engines since they offer significantly improved high temperature fatigue resistance, creep strength, and corrosion resistance [1–3]. It is generally known that microstructures are the strategic link between materials process and performance [4]. Directional solidification (DS) process has revolutionized the development of SC superalloys over the past few decades [5–7]. However, the basic problem of understanding and controlling microstructures during DS process is still a challenge. Dendrites as the predominant microstructural constituents of solidified superalloys largely determines the final serving properties of turbine blades or other castings [8–11]. To improve the performance, numerous researchers and technologists have worked on the dendritic structure of castings to develop their solidification behaviors in the respects of theory and experiment. Kurz and Fisher [12] proposed a general framework which related to tip radius, interface undercooling and primary arm spacing in alloy dendrite growth. This simplified model permitted a semi-quantitative prediction of the relationship between growth conditions and primary arm spacing. Subsequently, Trivedi and Kurz [13] systematically summarized the important aspects and theoretical models of dendrite growth, including in the undercooled melt and DS process. Normally, the microstructural scales of dendrites is always characterized by means of optical microscope (OM) or scanning electron microscope (SEM) technologies [14]. However, only the dendrite morphology in solid state can be observed, while the nucleation and growth processes of dendrites cannot be captured by using these experimental methods. In-situ observation techniques are increasingly used and developed to study the microstructure evolution. Some in-situ observation techniques have been employed for the real-time observation of dendrite growth during melting and solidification [15,16]. Qian et al. [17] reported a growing crystalline dendrite in a DS experiment on succinonitrile containing 1% acetone, the dendrites grew rapidly into a sidebranchlike feature according to the in-situ observation

* Corresponding author.
E-mail address: scjxqy@tsinghua.edu.cn (Q. Xu).

https://doi.org/10.1016/j.jcrysgro.2017.09.020
0022-0248/

results. A columnar-to-equiaxed transition (CET) of an Al-15 wt% Cu alloy in DS process, presented by Dong and co-workers [18], was tracked and recorded by using synchrotron X-radiation imaging technique, the CET process and equiaxed dendrites growth were described from the viewpoint of dendrite detachment. However, extensive experimental studies of in-situ observations were always focused on succinonitrile or low melting point alloy, the dendrite growth of superalloys was rarely mentioned because of the high melting point and density. The high temperature confocal laser scanning microscopy (HT-CLSM) as a powerful tool can offer a great capability for real-time and continuous observation of phase transformation at high temperatures. Gu et al. [19] investigated the microstructure evolution of M2, 100Cr6 and C38LTT steel grades by using HT-CLSM and high energy X-ray microtomography, and discussed the observations in terms of microstructural development and liquid fraction during heating. Attallah et al. [20] studied the initiation of incipient melting of primary γ′ in a Ni-base superalloy by using the HT-CLSM, and it was found that rapid heating prevented the dissolution of primary γ′. Although the HT-CLSM technique offers many advantages over classical experimental techniques, dendrite growth of in-situ observation in superalloy is still a challenge, due to the fact that it requires extremely high quality samples and complex operations.

In recent years, with the advancements of computer technology, numerical simulation as a powerful tool was used to investigate the dendrite growth during solidification [21–23]. Then, various simulation methods were emergence, and in particular phase field (PF) and cellular automaton (CA) approaches, which have permitted a validation of analytical theories as well as enabling predictions on dendrite growth and their evolution behavior. PF method is primarily rooted in continuum models of phase transitions that can precisely describe the dendrites interface and detailed morphology in two and even three dimensions [24,25]. However, large scale dendrites growth and 3-D polycrystalline solidification simulation using PF method are very difficult because of the need of enormous computational resources. CA method is another powerful computational approach that can reveal a wide range of micro/meso scale dendrite features, and has the advantage of a larger mesh size and much higher computational efficiency compared with PF method, and so it is extensively used in the investigation of dendrite growth [26–28]. In the last decade, important advances have been made in developing CA models and their algorithms of dendrite growth simulation. Initially, Rappaz and Gandin [29,30] proposed a CA coupled with finite element (FE) model in order to simulate the grain growth during solidification. Subsequently, there have been many studies on the simulation of DS dendrite growth and their evolution behavior using CA method. Wang et al. [31] developed a cellular automaton-finite difference (CA-FD) model to simulate solute diffusion controlled solidification of binary alloys, and found that perturbations significantly reduce the range of stable primary dendrite spacing. Pan et al. [32] built a 3-D sharp interface model for the quantitative simulation of dendrite growth, based on the local solutal equilibrium approach used to calculate the evolution of the S/L interface. Recently, Zhang et al. [33] presented a two-type directional dendrite growth model to realize the multi-scale simulation based on the CA-FD model considering macro DS parameters. However, most of studies mentioned above are 2-D or pseudo 3-D simulation for confining to calculation capability. Although some techniques such as the parallel computing and adaptive mesh refinement methods have been developed in order to enhance computational efficiency, large scale or 3-D dendrite growth simulation is still at the research stage.

The aim of this paper is to present a detailed study of dendrite growth in nickel-based superalloy using numerical simulation and in-situ observation technologies. A 3-D model are proposed to simulate dendrite growth, and the CA algorithm are also modified. Simulation parameters are calculated by dedicated software JMatPro, and the dendrite growth over a large scale in 2-D section and 3-D polycrystalline are simulated by the deterministic cellular automaton coupled with finite difference (DCA-FD) model. The instrumental device and the experimental procedure are described and the nucleation and growth during in-situ observation process are also analyzed. In addition, the samples are prepared a second time for dendritic morphology after HT-CLSM, and the simulation results are verified using these experimental results. Furthermore, the proposed model is also applied to the DS process to investigate the columnar dendrites growth.

2. Numerical modeling and experimental procedure

2.1. Solute diffusion coupling with temperature filed model

The dendrite growth is mainly controlled by solute redistribution and the temperature field during solidification. The solute distribution directly affects the dendrite morphology and dendrite arm spacing. Initially, the computational domain begins at a uniform composition, and the growing cells reject excess solute to its neighboring liquid cells with the solidification proceeding. Solute diffusion within the entire domain is then calculated coupled with the temperature field by Eq. (1) without considering nature and forced convection influence:

$$\frac{\partial C_i}{\partial t} = \nabla \cdot (D_i \nabla C_i) + C_i(1-k_0)\frac{\partial f_s}{\partial t} \tag{1}$$

where C is the composition with its subscript i denoting solid or liquid, D is the solute diffusion coefficient and k_0 is the equilibrium partition coefficient. The last terms on the right hand denotes the amounts of solute rejected due to the increment of solid fraction at the S/L interface.

At the interface of the liquid and solid, the partitioning of solute in the growing cell is determined by Eq. (2).

$$C_S = k_0 C_L \tag{2}$$

where C_S and C_L are the average solute concentrations of the solid and liquid, respectively, in the solid at the liquid/solid interface, k_0 is the equilibrium partition coefficient.

The solute concentration, C_L, in the liquid within a growing cell, is given by Eq. (3).

$$C_L = C_L^* - \frac{1-f_S}{2}\Delta x G_C \tag{3}$$

where C_L^* is the concentration in the liquid at the S/L interface, Δx is the cell size, G_C is the concentration gradient in the S/L interface. C_L^* can be determined from a linearized equilibrium phase relation:

$$C_L^* = C_0 + \frac{1}{m_L}(T^* - T_L + \Gamma\kappa f(\theta_i)) \tag{4}$$

where C_0 is the original solute concentration in the liquid, m_L is the liquidus slope, T^* is the actual interface equilibrium temperature, T_L is the equilibrium liquidus temperature at initial solute composition, Γ is the Gibbs-Thomson coefficient, κ is curvature of S/L interface and $f(\theta_i)$ is a anisotropy function can be described by Eqs. (5) and (6).

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

$$f(\theta_i) = \prod_{i=l,m,n}[1 + \varepsilon\cos(\delta_i\theta_i)] \tag{6}$$