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Free dendritic growth model incorporating interfacial nonisosolutal nature due to normal velocity variation

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Abstract: Considering both the effects of the interfacial normal velocity dependence of solute segregation and the local nonequilibrium solute diffusion, an extended free dendritic growth model was analyzed. Compared with the predictions from the dendritic model with isosolutal interface assumption, the transition from solutal dendrite to thermal dendrite moves to higher undercoolings, i.e., the region of undercoolings with solute controlled growth is extended. At high undercoolings, the transition from the mainly thermal-controlled growth to the purely thermal-controlled growth is not sharp as predicted by the isosolute model, but occurs in a range of undercooling, due to both the effects of the interfacial normal velocity dependence of solute segregation and the local nonequilibrium solute diffusion. Model test indicates that the present model can give a satisfactory agreement with the available experimental data for the Ni−0.7% B (mole fraction) alloy.

Key words: dendritic growth; interfacial nonisosolutal nature; modeling; binary alloy

1 Introduction

In past decades, numerous free dendritic growth models have been established, which include phase field models [1−3], models in the framwork of microscopic solvability theory [4−6] and models based on Ivantsov approach [7−21]. Phase field models adopt an order parameter, i.e., phase-field variable ϕ to describe the thermodynamic state of a local volume. This approach does not require tracking the solid−liquid interface and describes dynamical phenomena at the interface and in bulk phases through a single formalism. Microscopic solvability theory formulates dendritic growth problem as a single integro-differential equation and solves it without further hypotheses. The anisotropies of the interfacial energy and interfacial kinetics were taken into account, successfully. However, both of the phase field theory and microscopic solvability theory are very complicated, mathematically. It is not easy to be used for them, in practice. In contrast, the series of models based on Ivantsov approach received wide acceptance from materials scientists, due to its relative simplicity as well as the ability to describe the solidification with dendritic morphology.

During steady-state free dendritic growth, the paraboloid of revolution is a good approximation for the dendrite tip shape [22]. Based on this assumption, IVANTSOV [7,8] first obtained the exact solutions of the classical Fick diffusion equations for solute and thermal diffusions in bulk liquids. Subsequently, a series of free dendritic growth models were proposed by adopting the Ivanstov results, such as the well-known BCT model [12], the models developed by GALENKO and DANILOV [13,14] and SOBOLEV [15,16]. In BCT model, the thermodynamic driving force, the kinetic undercooling and Aziz's solute trapping model [23] were introduced to describe high Peclet conditions. However, this model could only deal with the deviation from local equilibrium state at the solid−liquid interface. By introducing the local nonequilibrium diffusion model, the dendritic growth models developed by GALENKO and DANILOV [13,14] and SOBOLEV [15,16] could describe the local nonequilibrium state both at the

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interface and in bulk liquids. Recently, WANG et al [20] further extended the series of models to concentrated multi-component alloys. In all of these models, however, it is assumed that the interface is isothermal and isosolutal.

During steady-state growth, the normal velocity varies along the dendritic interface. This variation would lead to different solute partitioning along the interface and further lead to a nonisosolutal solid−liquid interface. It is also well known both from phase field and experiments, that the solute content in a dendritic structure has a typical appearance, i.e., high concentration along the stem and low concentration on both sides. Therefore, it is significant to analyze the effect of the interfacial normal velocity dependence of solute segregation on the dendritic solidification behavior. Recently, a generalized free dendritic growth model was developed by solving the classical Fick diffusion equation exactly under the boundary condition of nonisothermal and nonisosolutal interface [24]. However, the effect of local nonequilibrium solute diffusion in bulk liquid was not taken into account. In the present work, a relatively simple method was proposed to analyze both the effects of the interfacial normal velocity dependence of solute segregation and the local nonequilibrium solute diffusion. An experimental comparison with the available experimental data for the Ni−0.7%B (mole fraction) alloy was also made.

2 Model

In this section, two independent variables were introduced to describe the dendritic morphology during steady state solidification. Based on this interfacial morphology, the solute trapping model recently developed by LI and SOBOLEV [25] was outlined. Then taking into account the interfacial driving force, an interfacial response function was proposed, approximately. From this interfacial response function, the tip radius of curvature was derived. Finally, an extended free dendritic growth model was obtained for binary alloys, which could deal with both the interfacial normal velocity dependence of solute segregation and the local nonequilibrium solute diffusion.

2.1 Extended solute trapping model

During steady-state solidification, the dendritic morphology could be approximated by a paraboloid of revolution [22]. For describing the interfacial morphology with the paraboloid of revolution uniquely, it is required mathematically to introduce the radius of curvature (R) at the dendrite tip. This parameter has been widely adopted in previous dendritic models [9−21]. In the present work, taking into account the interfacial normal velocity dependence of solute partitioning, it is not enough to only adopt the parameter R. Here, an angle (θ) is introduced. The normal direction at an interface element makes the angle θ with respect to the growth axis. For steady-state growth at a given interface migration velocity V (i.e., tip velocity), there is a critical value of the angle θ. This critical angle θ, i.e., the maximum angle, is marked by $\theta_{\max}$. For $\theta \geq \theta_{\max}$, the solid−liquid interface becomes unstable and the secondary dendrite arm and necking phenomenon may appear. The present model focuses on the range of $0 \leq \theta \leq \theta_{\max}$, which corresponds to the shape preserving part of the dendritic interface. Therefore, considering the interfacial normal velocity dependence of solute segregation, one should use both the parameter R and the angle $\theta_{\max}$ to describe the steady-state shape and the boundary.

Along the dendritic interface from the tip (θ=0) to the root ($\theta=\theta_{\max}$), the normal velocity V_n decreases, which could be described by $V_n(\theta)=V\cos\theta$ due to the shape preserving condition. The normal velocity $V_n(\theta)$ can be regarded as the effective velocity which controls the solute redistribution at the interface element marked by angle θ. Introducing this dependence of V_n on θ into the solute trapping model proposed by SOBOLEV [15,16], the solute partition coefficient K could be further described as [25]

$$K(V,\theta)=\begin{cases}\dfrac{K_E(1-V^2\cos^2\theta/V_D^2)+V\cos\theta/V_{DI}}{(1-V^2\cos^2\theta/V_D^2)+V\cos\theta/V_{DI}}, & V\cos\theta<V_D \\ 1, & V\cos\theta\geq V_D\end{cases} \tag{1}$$

where K_E is the equilibrium partition coefficient, V_{DI} is the interface diffusive speed and V_D is the bulk liquid diffusive speed.

In order to analyze the effect of the interfacial normal velocity dependence of solute segregation on the dendritic solidification behavior, it is useful to calculate the average of partition coefficient $\overline{K}(V)$ from the tip to the root of the dendrite. For the interface approximated by a paraboloid of revolution, $\overline{K}(V)$ could be given as follows [25]:

$$\overline{K}(V)=\begin{cases}\dfrac{3\int_0^{\theta_{\max}}K(V,\theta)\exp(3\theta)\mathrm{d}\theta}{\exp(3\theta_{\max})-1}, & V\cos\theta_{\max}<V_D \\ 1, & V\cos\theta_{\max}\geq V_D\end{cases} \tag{2}$$

2.2 Interfacial response function

In previous models, the driving force on solidification, i.e., the effective driving free energy ΔG_{EFF} was calculated with the values for liquid solute