A new analytical model for the growth rate of dendrite tips

Xiaohui Ao, Huanxiong Xia*, Jianhua Liu, Qiyang He, Shengxiang Lin
School of Mechanical Engineering, Beijing Institute of Technology, Beijing, China

*Corresponding author e-mail: hxia@bit.edu.cn

Abstract. It’s well known that the driving forces of dendrite growth in metal solidification typically include temperature undercooling, constitutional undercooling, and curvature undercooling, and these undercoolings are usually computed independently by their corresponding local temperature, concentration, and curvature in a model. This paper derived a new formula only depending on the temperature undercooling based on the dynamic equilibrium relationship and the Ivantsov function for computing the growth rate of dendrite tips at the equilibrium state. By taking the derivative of this formula to find the maximum growth rate, an almost constant ratio of the curvature undercooling to the temperature undercooling was found, specifically, the ratio is in the range of 0.507 to 0.524 corresponding to the temperature undercooling of 4 to 10 K. The analytical result was validated by the numerical simulations of the solidification of Inconel 718 alloy with different temperature undercoolings by using a cellular-automata method. The numerical results suggested a ratio of 2/3 of the curvature undercooling to the temperature undercooling for the given Inconel 718 alloy.

1. Introduction
Precisely predicting and controlling the microstructure of metals and alloys during solidification processes has attracted amounts of effort. The dendrite growth during a solidification process is an extremely complex physical behavior, which needs to consider the influences of temperature, concentration, curvature, grain orientation, interface energy anisotropy, and other factors [1-2]. Many deterministic and stochastic models have been developed to simulate the growth of dendrites, such as the phase-field method [3-4], cellular automata [5], and Monte Carlo method [6], etc. The Cellular Automata (CA) model is widely used to simulate solidification processes in science and engineering due to its high computational efficiency and relatively simple physical principles.

As dendrites grow under the coupling of temperature field and concentration field, the analytical theories that are used to deal with steady-state kinetics cannot take an insight into the dynamic evolution of dendrite growth. It is a big challenge that how to capture the front of the solid/liquid (SL) interface and determine its growth velocity. Based on the principle of interface stability, Kurz et. Al [7] proposed the KGT model to calculate the growth rate of dendrite tips and the simulation results could well present the phenomenon of columnar crystal competition and equiaxed crystal growth. A dimensionless Lipton-Glicksman-Kurz (LGK) model for the growth of equiaxed dendrites of alloys under a small Peclet number was developed by Lipton [8]. Zhu and Stefanescu [9] proposed a method to calculate the dynamics of dendrite growth based on the balance of interfacial solutes, the results indicated that dendrite growth is driven by the difference between the local concentration and the equilibrium concentration of the liquid-phase composition. A new Zigzag trapping rule was proposed...
to simulate the morphology of dendrite growth during the solidification of pure materials by Wei et. al [10]. A modified eccentric algorithm presented in simulating the dendrite growth under different preferred growth orientations can be found in [11-13].

This work is devoted to taking an insight into the dynamic relationship of the temperature, composition, and curvature on the growth rate of dendrite tips and theoretically analyzing the ratio of the curvature undercooling to the temperature undercooling. Furthermore, the growth rate of dendrite tips was given analytically based on the thermodynamic equilibrium and Ivantsov function.

2. Analytical derivation and simulation validation

According to the thermodynamic equilibrium at the front of the solid-liquid interface, a relationship between temperature, concentration and interface curvature can be expressed as[14]:

$$\Delta T = m(C_0 - C^*) + \Gamma \kappa f(\theta, \theta_0)$$

(1)

where $\Delta T$ and $C^*$ are the temperature undercooling and the liquid-phase concentration at the solid-liquid interface, respectively, $C_0$ and $m$ are the initial equilibrium concentration and liquidus slope of the original alloy, respectively, $\Gamma$ the Gibbs Thomson coefficient, and $\kappa$ the mean curvature.

Assume $\omega$ is the ratio of the curvature undercooling to the temperature undercooling as:

$$\omega = \frac{\Gamma \kappa f(\theta, \theta_0)}{\Delta T}$$

(2)

Then, the radius of the dendrite tip can be given as:

$$R = \frac{2\Gamma f(\theta, \theta_0)}{\omega \Delta T}$$

(3)

The solute supersaturation is equal to Peclet function value, which is defined as:

$$\Omega = \frac{C^* - C_0}{C^*(1 - k_0)} = Iv(Pe)$$

(4)

where the Peclet number $Pe = RV/2D$ ($V$ is the growth rate of dendrite tips, $D$ is the diffusion coefficient of the solute). The Peclet function can be obtained by solving the solution steady-state diffusion equation at the dendrite tip with an assumption that the solid-liquid interface is isothermal or equal-concentration parabola by Ivantsov as:

$$Iv(Pe) = Pe \exp(Pe) \int_{-\infty}^{+\infty} \frac{\exp(-z)}{z} dz, \quad (5)$$

The Ivantsov function is usually used with its first-order approximation as follows:

$$Iv(Pe) = \frac{Pe}{Pe + 1}, \quad (6)$$

Combined equations (1)-(6), the relationship between the growth rate of the dendrite tip and the temperature undercooling can be written as:

$$V = \frac{\omega D \Delta T^2}{\Gamma f(\theta, \theta_0)[mC_0(k_0 - 1)/(1 - \omega) - k_0 \Delta T]}$$

(7)

Eq. (7) yields a limit of the temperature undercooling:

$$\Delta T \leq \frac{mC_0(k_0 - 1)}{k_0(1 - \omega)}$$

(8)

By taking the derivative of eq. (7) to the ratio $\omega$ to find the maximum growth rate, $dV/d\omega=0$, the optimal ratio is obtained as:

$$\omega_{opt} = 2 + \sqrt{a^2 - a + 1} - a \over 3$$

(9)

where $a=mC_0(k_0-1)/(k_0\Delta T)$. For Inconel 718 alloy, the dependence of the optimal ratio $\omega_{opt}$ on the temperate undercooling $\Delta T$ is shown as in Figure 1. It can be seen that the optimal ratio $\omega_{opt}$ changes a little in the range of 4-10 K of the temperate undercooling.
Figure 1. Dependence of the optimal ratio $\omega_{\text{opt}}$ on the temperate undercooling $\Delta T$ for Inconel 718 alloy.

To validate the analytical model of the growth rate of dendritic tips, a few simulations of Inconel 718 alloy with different temperature undercoolings were carried out. For the details of the model of these simulations, please see our previous work [15]. The material properties of Inconel 718 alloy used in the simulations are listed in Table 1.

Table 1. Material parameters of Inconel 718 alloy.

| Property and symbol                              | Value  | Ref. |
|------------------------------------------------|--------|------|
| Liquidus temperature $T_l$ (K)                 | 1609   | [16] |
| Solidus temperature $T_s$ (K)                  | 1533   | [16] |
| Initial solute concentration $C_0$ (wt.%      | 5.0    | [17] |
| Liquidus slope $m$ (K·wt.%$^{-1}$)             | -10.5  | [17] |
| anisotropy coefficient $\varepsilon$           | 0.2    | [17] |
| Partition coefficient $k_0$                    | 0.48   | [17] |
| Gibbs-Thomson coefficient $\Gamma$ (K·m)       | $2.4 \times 10^{-7}$ | [18] |
| Liquid diffusion coefficient $D_l$ (m$^2$·s$^{-1}$) | $3 \times 10^{-9}$ | [18] |

Figure 2. The numerical simulation results of the evolution of curvature undercooling at the dendrite tip under different temperature undercoolings. The applied temperature undercoolings are 5 K, 7.5 K, and 10 K, respectively.

Figure 2 shows the relationship between temperature undercooling and curvature undercooling. The results indicate that the ratio of the curvature undercoolings to the corresponding applied temperature undercoolings are all about 2/3, namely $\omega \approx 2/3$. The error of $\omega$ between the simulated and the analytical results may result from numerical accuracy, Ivantsov functions, and others.
3. Conclusion

In this paper, an analytical model calculating the growth rate of dendrite tips by only using the temperature undercooling was developed based on the dynamic equilibrium relationship of temperature, composition, and curvature and the Ivantsov function. The optimal ratio of the curvature undercooling to temperature undercooling that allows the growth rate of dendrite tips is maximum is almost consistent with this ratio obtained from the simulations of the free growth of dendrite tips. The exact values of the ratio from the analytical and simulated results currently do not show a perfect agreement with each other, which could result from the rotating-parabola hypothesis for the tip profile of the dendrite under a larger undercooling. Overall, this model provides a new way to calculate the growth rate of dendrite tips and a new perspective to interpret the dynamics of the growth rate of dendrite tips.

4. Acknowledgments

This work was financially supported by the National Major Research Program of China (No. 2018YFB1105304) and the Youth Academic Launch Program of Beijing Institute of Technology.

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