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Free dendritic growth model based on nonisothermal interface and microscopic solvability theory

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Abstract: Considering both the effect of nonisothermal nature of the solid/liquid interface and the microscopic solvability theory (MicST), a further improved version of free dendritic growth model for pure materials was proposed. Model comparison indicates that there is a higher temperature at the tip of dendrite predicted by the present model compared with the corresponding model with the isothermal solid/liquid interface assumption. This is attributed to the sidewise thermal diffusion, i.e. the gradient of temperature along the nonisothermal interface. Furthermore, it is indicated that the distinction between the stability criteria from MicST and marginal stability theory (MarST) is more significant with the increase of bath undercoolings. Model test also indicates that the present model can give an agreement with the available experimental data. It is finally concluded that the nonisothermal nature of the solid/liquid interface and the stability criterion from MicST should be taken into account in modeling free dendritic growth.

Key words: dendrite; solidification; modeling; interface; microscopic solvability theory

1 Introduction

The free dendritic growth in an undercooled melt has attracted focused attention in the research of solidification experiment as well as theory in the past decades [1−6]. To model free dendritic growth, three parts must be treated, including interface kinetics, thermal or solutal transport in the bulk liquid and morphological stability for the solid/liquid (S/L) interface. For the interface kinetics, Turnbull's collision-limited growth model [7] is commonly used, for both metals and alloys, to describe an interface responce function, i.e. a relationship among the interfacial migration velocity, temperature and compositions of solid and liquid phases. To describe the thermal and solutal transport in liquid ahead of the S/L interface, the classical Fick diffusion equation or the extended hyperbolic diffusion equation was used [8−16]. The first attempt was made by IVANTSOV [8,9] to obtain an exact solution with the assumption of isothermal and isosolutal S/L interface of a paraboloid of revolution. Based on the Ivantsov's result, a series of free dendritic growth models were proposed [11−14]. Recently, eliminating the isothermal and isosolutal S/L interface assumption, LI et al [17,18] have further obtained the exact solution of steady state Fick diffusion equation, successfully. In reality, the curvature and normal velocity are variable along the S/L interface under the steady state growth condition. This means that the interface is nonisothermal and nonisosolutal (anisotropic). Therefore, taking into account the anisotropic nature of the S/L interface is meaningful.

All of these free dendritic growth models mentioned above adopted marginal stability theory (MarST) [19−25] to deal with the morphological stability for S/L interface. MarST has been widely adopted by materials scientists and engineers, due to its ability of giving an agreement with experiment data [24,25]. However, it should be noted that MarST has its theoritical limitations. A steady state parabolic shape does not exist in the absence of anisotropy [26,27]. That is to say, the interfacial anisotropy (at least the surface energy anisotropy) is required to guarantee a steady state

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parabolic shape of S/L interface. In MarST, the hypothesis of isotropic S/L interface is made, which leads to the unphysical results, e.g. yields tip splitting. Taking into account the interfacial anisotropy, microscopic solvability theory (MicST) [26−31] has also been developed to describe the morphological stability of S/L interface, including the selected mode for rapidly growing needle-like dendrite.

In the present work, a more improved version of the free dendritic growth model was proposed by considering both MicST and the effect of nonisothermal nature of the S/L interface. As first attempt, pure materils were focused. A comparison of the present model (nonisothermal dendritic growth model with MicST) with the nonisothermal dendritic growth model with MarST and the isothermal dendritic growth model with MicST was made. Furthermore, a model comparison with the available experiment data was also made.

2 Model

In this section, the interface response function which can deal with the nonisothermal nature of the S/L interface was firstly described. Then, taking the interface response function as a boundary condition of the thermal diffusion equation, an exact solution was obtained, which can describe the tip temperature of the nonisothermal interface. Finally, the stability criterion from MicST was introduced to replace the MarST.

2.1 Interface response function

During steady state dendritic growth, the morphology of S/L interface could be approximated by a paraboloid of revolution. It will be convenient to use a parabolic coordinate system (α, β, θ), which makes α=1 represent the S/L interface [17,18]. At different points of the S/L interface (with different values of β), the interfacial curvature ($1/r(\beta)$) and normal velocity ($V_n(\beta)$) are different. This implies that the curvature undercooling (ΔT_r) and kinetic undercooling (ΔT_k) are variable along the interface. Thus, the S/L interface is nonisothermal in reality. Taking into account the nonisothermal nature of the S/L interface, the interfacial responce function can be extended as [32]

$$T_L(1,\beta)=T_m-\frac{\Gamma}{r}\frac{2+\beta^2}{(1+\beta^2)^{3/2}}-\frac{V}{\mu_0}\frac{1}{(1+\beta^2)^{1/2}} \quad (1)$$

where $T_L(1, \beta)$ is the interfacial temperature, T_m is the melting point, Γ is the Gibbs−Thompson coefficient, μ_0 is the kinetic coefficient, r is the radius of curvature at the tip, and V is the velocity of the dendrite growth in the axial direction. Equation (1) is reduced to the one commonly used in previous models [1] by setting β=0.

2.2 Thermal transport

For free dendritic growth in undercooled melts, the interfacial temperature is higher than that in liquid far from the interface due to the release of the latent heat. Therefore, there must be thermal transport in the liquid ahead of S/L interface to guarantee a steady state growth. Ignoring thermal diffusion in the solid, the thermal transport phenomenon in the liquid can be described by the classical Fick diffusion equation as [13]

$$\left(D_T\nabla^2-\frac{\partial}{\partial t}\right)T_L(\alpha,\beta)=0 \quad (2)$$

where $T_L(\alpha, \beta)$ is the actual temperature in the liquid, and D_T is the thermal diffusivity in the liquid. For mathematical convenience, a new temperature field $U_L(\alpha, \beta)$ in the liquid is defined by [17]

$$U_L(\alpha,\beta)=T_L(\alpha,\beta)-T'_L(\alpha) \quad (3)$$

where $T'_L(\alpha)$ is the temperature field obtained by fictitious problem of an isothermal interface (Ivantsov condition), which is described as [8,9]

$$T'_L(\alpha)=\frac{\Delta H}{c_p}p_t e^{p_t}E_1(p_t\alpha^2)+T_\infty \quad (4)$$

where ΔH is the latent heat of fusion, c_p is the specific heat capacity, E_1 is the exponential integral function, T_∞ is the temperature of the undercooled melt far from the interface and p_t is the thermal Peclet number defined by $p_t=rV/(2D_T)$. Particularly, $T'_L(\alpha)$ is equal to ΔT_t+T_∞ at α=1 (the S/L interface), where ΔT_t is the thermal undercooling defined by $\Delta T_t=\mathrm{Iv}(p_t)\Delta H/c_p$ and $\mathrm{Iv}(p_t)$ is Ivantsov function [5].

With the parabolic coordinate system (α, β, θ) and the definition of $U_L(\alpha, \beta)$ described by Eq. (3), Fick diffusion equation, Eq. (2), can be rewritten as follows [17]:

$$\frac{\partial^2 U_L}{\partial\alpha^2}+\left(\frac{1}{\alpha}+2p_t\alpha\right)\frac{\partial U_L}{\partial\alpha}+\frac{\partial^2 U_L}{\partial\beta^2}+\frac{1}{\beta}\frac{\partial U_L}{\partial\beta}=0 \quad (5)$$

In this equation, a term $-2p_t\beta\partial U_L/\partial\beta$ is neglected under the condition $1/\beta\gg 2p_t\beta$. This condition is reasonable since the solidification behavior at tip of the dendrite (β=0) is only influenced by the regions in the vicinity of $\beta\approx 0$.

Ignoring solid temperature gradient, the thermal transport balance could be described by

$$V\Delta H=-\frac{K_L}{r}\partial T_L(\alpha,\beta)/\partial\alpha|_{\alpha=1} \quad (6)$$

where K_L is the thermal conductivity of the liquid. The thermal diffusion equation (Eq. (5)), combined with the boundary conditions (Eqs. (1) and (6)), could be solved exactly to obtain the description of temperature field $U_L(\alpha, \beta)$, which further gives the following relationship at the tip (β=0) [17]:

$$\Delta T=\frac{\Delta H}{c_p}\mathrm{Iv}(p_\mathrm{t})+\frac{V}{\mu_0}N_1(p_\mathrm{t})+\frac{2\Gamma}{r}N_2(p_\mathrm{t}) \tag{7}$$

where ΔT is the bath undercooling defined by $T_\mathrm{m}-T_\infty$, and the parameters $N_1(p_\mathrm{t})$ and $N_2(p_\mathrm{t})$ are defined by

$$N_1(p_\mathrm{t})=\mathrm{Iv}(p_\mathrm{t})\int_0^\infty \mathrm{e}^{-\lambda}\frac{\Phi\left(1+\dfrac{\lambda^2}{4p_\mathrm{t}},2,p_\mathrm{t}\right)}{\Phi\left(1+\dfrac{\lambda^2}{4p_\mathrm{t}},1,p_\mathrm{t}\right)}\mathrm{d}\lambda \tag{8}$$

$$N_2(p_\mathrm{t})=\mathrm{Iv}(p_\mathrm{t})\int_0^\infty \mathrm{e}^{-\lambda}\frac{(1+\lambda)}{2}\frac{\Phi\left(1+\dfrac{\lambda^2}{4p_\mathrm{t}},2,p_\mathrm{t}\right)}{\Phi\left(1+\dfrac{\lambda^2}{4p_\mathrm{t}},1,p_\mathrm{t}\right)}\mathrm{d}\lambda \tag{9}$$

where $\Phi(a,b,Z)$ is the confluent hypergeometric function of the second kind. If the parameters $N_1(p_\mathrm{t})$ and $N_2(p_\mathrm{t})$ equal unity, the relationship, Eq. (7), reduces to the one used by models with isothermal S/L interface assumption.

2.3 Morphological stability criterion

Based on the thermal diffusion field with a boundary condition of nonisothermal interface, the relationship, Eq. (7), has been obtained, which gives a correlation between the tip radius of curvature r and the interfacial migration velocity V at a given bath undercolling ΔT. In order to uniquely determine solidification behavior of steady state dendritic growth, another relationship should be established. A morphological stability criterion of S/L interface can give the additional information. LANGER and MULLER-KRUMBHAAR [33] introduced a stability criterion of the form Vr^2=constant for small Peclet numbers and a scaling parameter σ defined by

$$\sigma=\frac{2d_0D_\mathrm{T}}{r^2V}=\frac{d_0}{rp_\mathrm{t}} \tag{10}$$

where d_0 is the capillary length determined by $d_0=\Gamma c_p/\Delta H$.

According to Ref. [33], the radius of curvature r at the dendritic tip can be approximated by the shortest perturbed wavelength λ_s ($\lambda_\mathrm{s}=2\pi/\omega$, ω is the angular velocity). Placing sinusoidal perturbation $Z=\delta(t)\sin(\omega x)$ on the planar S/L interface and following the standard stability criterion procedure of the linear analysis of morphological stability, MarST gives the following stability criterion [19]:

$$\sigma=\sigma^*\xi_\mathrm{t}=\sigma^*\{1-[1+(\sigma^*p_\mathrm{t}^2)^{-1}]^{1/2}\} \tag{11}$$

where σ^* is a constant ($\sigma^*=1/(4\pi^2)$), and ξ_t is a medium variable. This theory has its theoritical limitations just as aforementioned that it makes the hypothesis of an isotropic S/L interface. A steady state parabolic shape does not exist under this condition [26,28]. That is to say, the interfacial anisotropy, at least the surface energy anisotropy, is required to guarantee a steady state parabolic shape of S/L interface. Taking into account the surface energy anisotropy, MicST successfully deals with the problem of morphological stability and gives the stability criterion as follows [30]:

$$\sigma=\sigma_0a_\mathrm{d}^{7/4}\xi_\mathrm{t}=\sigma_0a_\mathrm{d}^{7/4}\frac{1}{(1+a_1\sqrt{a_\mathrm{d}}\,p_\mathrm{t})} \tag{12}$$

where a_d is the surface anisotropy stiffness, σ_0 is the selection constant, and a_1 is a constant defined by σ_0 ($a_1=(8\sigma_0/7)^{1/2}(3/56)^{3/8}$).

Therefore, one should take the stability criterion, Eq. (12), to replace the stability criterion from MarST, i.e. Eq. (11), even though it has been widely used by materials scientists [19−25]. Up to now, considering both MicST and the effect of nonisothermal nature of the S/L interface, the entire free dendrite growth model has been described. It contains two independent equations, Eqs. (7) and (12). Solving these two equations numerically, one can determine the interfacial migration velocity V and the radius of curvature r at the tip, and further obtain the temperature distribution $T_\mathrm{L}(1,\beta)$ along the S/L interface at any given bath undercooling ΔT.

3 Results and discussion

A model comparison was carried out to analyze the effect of nonisothermal interface (Section 3.1) and the difference between the present nonisothermal model with MicST and the previous nonisothermal model with MarST (Section 3.2). Finally, an experimental comparison was made (Section 3.3). The numerical results are shown in Figs. 1−5, by application to the pure materials white phosphorous. The thermophysical data, used in the present calculation, are listed in Table 1.

3.1 Effect of nonisothermal interface

The interfacial temperatures as functions of the normalized bath undercooling for the nonisothermal model and isothermal model are shown in Fig. 1. The temperatures $T_\mathrm{L}(1,\beta)$ at β=0 (the tip of dendrite) and β=0.5 are given for the nonisothermal model due to the variation in temperature along the interface. It also gives the interfacial temperature $T'_\mathrm{L}(1)$, i.e. the tip temperature predicted by the isothermal model due to the isothermal assumption of the S/L interface. It is indicated that the interface temperature $T_\mathrm{L}(1,0.5)$ is higher than the tip temperature $T_\mathrm{L}(1,0)$ predicted by the nonisothermal model. In order to show this nonisothermal nature of the S/L interface more clearly, the temperatures along the interface at different values of β are given by the insert in Fig. 2, at the normalized bath undercooling $\Delta\Theta$=0.7 as an example. It can be seen that there is a gradient of temperature along the interface and the temperature increases along the interface from the tip to the root. This implys that the temperature is increasing along the interface from the tip to the root. This gradient would result in an extra sidewise thermal diffusion which further leads to the increase of the tip temperature. Therefore, a higher temperature at the tip is predicted by the present nonisothermal model compared with the isothermal model (see Fig. 1) because there is no additionally sidewise thermal diffusion (see the insert in Fig. 2). In Fig. 2, we also define $\Delta T_{\mathrm{model}} = T_{\mathrm{L}}(0,1) - T'_{\mathrm{L}}(1)$ as the difference of temperature between the tip temperatures pridected by the two models and $\Delta T_{\mathrm{i}}=T_{\mathrm{L}}(1,0.5)-T_{\mathrm{L}}(1,0)$ to denote the gradient of temperature along the nonisothermal interface. It is

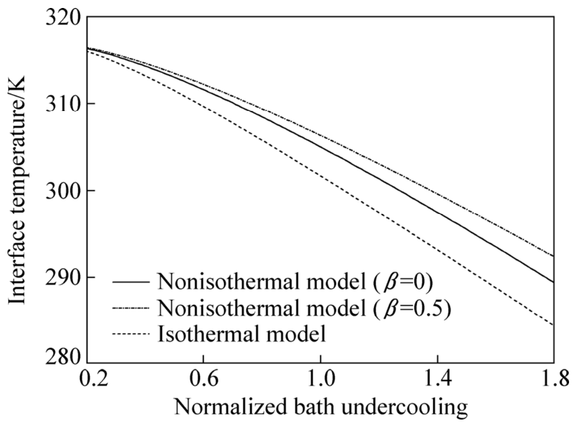

Fig. 1 Evolution of interfacial temperature as function of normalized bath undercooling $\Delta\Theta$, defined by $\Delta\Theta=\Delta Tc_p/\Delta H$ with MicST

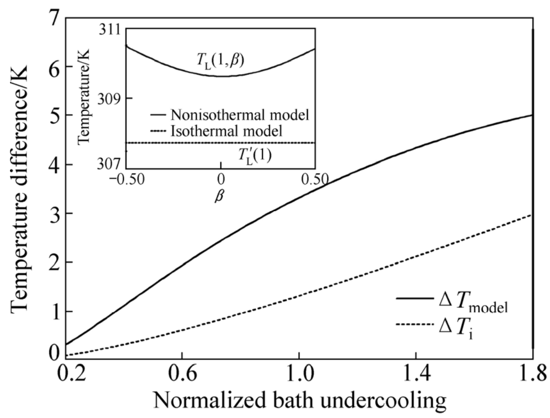

Fig. 2 Temperature differences $\Delta T_{\mathrm{model}}$ and ΔT_{i} as functions of normalized bath undercooling (The insert shows the temperature profiles $T_{\mathrm{L}}(1,\beta)$ and $T'_{\mathrm{L}}(1)$ along the interface at $\Delta\Theta$=0.7. $\Delta T_{\mathrm{model}}$ is the difference between the tip temperatures calculated by the nonisothermal and isothermal model, defined by $T_{\mathrm{L}}(1,0)- T'_{\mathrm{L}}(1)$, and ΔT_{i} is defined by the temperature difference $T_{\mathrm{L}}(1,0.5)-T_{\mathrm{L}}(1,0)$)

indicated that with the increase of the normalized bath undercooling, the difference ΔT_{i} increases and the difference $\Delta T_{\mathrm{model}}$ also increases. This further confirms that the higher temperature at the tip predicted by the present nonisothermal model is caused by the variation in temperature along the interface, i.e. the gradient of temperature along the nonisothermal interface.

3.2 Model comparison on MarST and MicST

In order to compare the effects of MarST and MicST on free dendritic growth models, dendrite tip radius of curvature as a function of the normalized bath undercooling is shown in Fig. 3. By comparing Eq. (11) with Eq. (12), one of the main distinctions lies in the expression of the paramter ξ_{t}, which are shown in Fig. 4 for both MarST and MicST. At relatively low bath undercoolings $\Delta\Theta$, the difference of radius of curvature predicted by the two models is relatively small in comparison with that at high $\Delta\Theta$ (Fig. 3). This can be explained as follows. When the bath undercooling is very small, Peclet number is small enough to meet the condition $d_0 \ll r \ll l$, where l is the diffuson length defined as $2D_{\mathrm{T}}/V$. According to Ref. [33], the stability criterion of the form Vr^2 = constant is reasonable for small Peclet number and the scaling parameter σ can be rewritten as $\sigma=[\lambda_{\mathrm{s}}/(2\pi r)]^2$, where $\lambda_{\mathrm{s}}=2\pi\sqrt{ld_0}$ is the shortest warelength of disturbance which would cause a plane interface to suffer a MULLINS-SEKERKA instability [24]. Under the condition $d_0 \ll r \ll l$, LANGER and MULLER-KRUMBHAAR [33] concluded that the stability of dendrite tip interface can be maintained with $r \equiv \lambda_{\mathrm{s}}$. When the Peclet number is small enough, ξ_{t} for both MarST and MicST would be approximate to unit as shown in Fig. 4. Thus, the stability criteria from MarST and MicST, Eqs. (11) and (12) are reduced to Vr^2=constant, given by LANGER and MULLER-KRUMBHAAR [33] at relatively low $\Delta\Theta$. However, as shown in Figs. 3 and 4, with increase of $\Delta\Theta$, the distinction between the stability criteria from MarST and

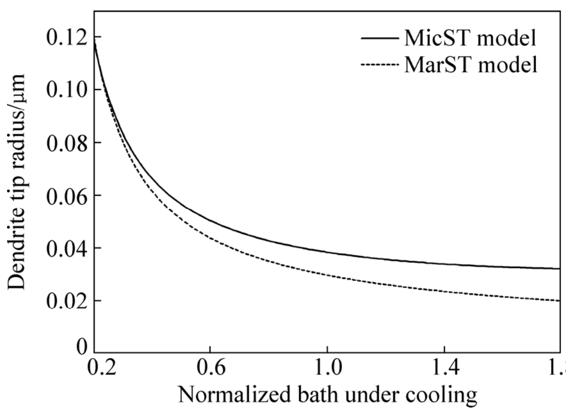

Fig. 3 Dendrite tip radius of curvature as function of normalized bath undercooling (Using nonisothermal model)

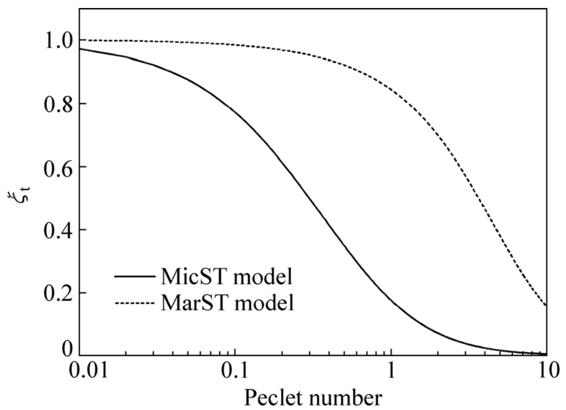

Fig. 4 Parameter ξ_t as function of Peclet number using nonisothermal model

MicST is more remarkable. This significant distinction should be taken into account in modeling free dendrtic growth.

3.3 Experimental comparison

An experimental comparison for the interfacial migration velocity V versus the normalized bath undercooling is shown in Fig. 5. The kinetic coefficient μ_0 and the Gibbs−Thompson coefficient Γ were treated as fitting parameters in their reasonable range. And σ_0 as the selection constant was also adjusted so that the experimental data can be fitted well. An agreement of the prediction from the present model with the experiment data is obtained at $\Delta\Theta\leq1.2$. The deviation from experimental data at high undercooling may be attributed to the following two reasons. Firstly, some parameters may be changed with the variation of temperature, such as D_T, Γ and μ_0. For example, with the increase of $\Delta\Theta$, the solidification velocity V increases. When V is high enough the defect in materials increases during solidification, so the entropy of solid will be heightened.

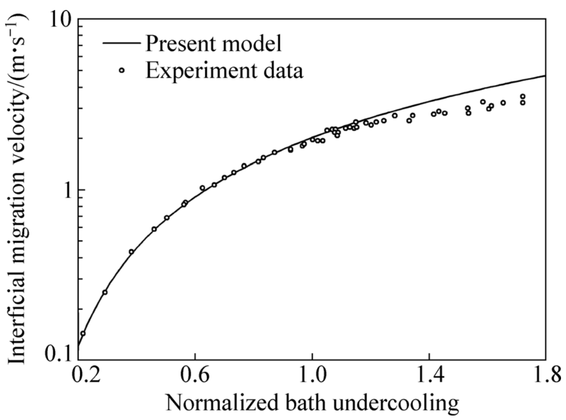

Fig. 5 Interfacial migration velocity as function of normalized bath undercooling calculated by present nonisothermal model with MicST and available experimental data for white phosphorus [33]

Table 1 Thermodynamic parameters for white phosphorus used in model computation [17]

Parameter	Value
Melting point of P_4, T_m/K	317.1
Hypercooling, $(\Delta H\cdot c_p^{-1})$/K	25.6
Capillarity constant, Γ/(K·m)	4.277×10^{-9}
Thermal diffusivity, D_T/($m^2\cdot s^{-1}$)	1.302×10^{-7}
Kinetic coefficient, μ_0/($m\cdot s^{-1}\cdot K^{-1}$)	0.17
Surface energy stiffness, a_d	0.15
Capillary length, d_0	2.073×10^{-8}
Selection constant, σ_0	80

This means that the effective thermodynamic driving force will be reduced and finally the interfacial migration velocity V would become lower. This corresponds to a lower value of the kinetic parameter μ_0 at high $\Delta\Theta$. Secondly, at high $\Delta\Theta$ the S/L interface experiences from a dendrite to a scalloped structure. That is to say, the morphological stability with the paraboloid of revolution cannot be maintained, namely, it is not predictable using the present model.

4 Conclusions

(1) A free dendritic growth model was proposed for pure materials by considering both the effect of nonisothermal nature of the S/L interface and the microscopic solvability theory (MicST). Comparative analysis indicates that the present model provides an agreement with the available experimental data for white phosphorus.

(2) Model comparison between the present model (nonisothermal dendritic growth model with MicST) and the dendritic growth model with MicST and the isothermal S/L interface assumption indicates that there is a higher temperature at the tip predicted by the present nonisothermal model. This is due to the variation in temperature along the interface, i.e. the gradient of temperature along the nonisothermal interface.

(3) Model comparison between the present model (nonisothermal dendritic growth model with MicST) and the previous nonisothermal dendritic growth model with the marginal stability theory (MarST) indicates that the distinction between MarST and MicST disappears if Peclet number is small enough, and with the increase of bath undercoolings (Peclet number) the distinction between the stability criteria from MarST and MicST is more significant. This should be taken into account in modeling free dendritic growth.

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基于界面非等温特性以及微观可解性理论的自由枝晶生长模型

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摘 要：在同时考虑固/液界面非等温性质的影响与微观可解性理论(MicST)的情况下，提出一个更加完善的纯物质自由枝晶生长模型。模型比较结果表明：与相应假设的等温固/液界面模型相比，本文作者提出的模型预测的枝晶尖端温度更高，这归因于沿着非等温界面的侧向热扩散，即温度梯度。此外，随着过冷度的增大，MicST 与边缘稳定性理论(MarST)给出的稳定性判据间的差异变得更加明显。模型测试结果表明：本模型的预测结果与实验数据吻合较好。因此，在自由枝晶生长建模中必须考虑固/液界面非等温性质的影响与 MicST 给出的稳定性判据。

关键词：枝晶；凝固；建模；界面；微观可解性理论

(Edited by Wei-ping CHEN)