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3D anisotropy simulation of dendrites growth with phase field method

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Abstract: The anisotropy problem of 3D phase-field model was studied, and various degrees of anisotropy were simulated by numerical calculation method. The results show that with the change of interface anisotropy coefficients, from smooth transition to the appearance of angle, equilibrium crystals shape morphology has a critical value, and 3D critical value is 0.3. The growth of dendrites is stable and the interface is smooth when it is less than critical value; the interface is unstable, rolling edge appears and the growth is discontinuous when it is more than critical value. With the increase of anisotropy coefficients, the dendrites grow faster under the same condition.

Key words: anisotropy; dendrite growth; crystal morphology; phase field method

1 Introduction

The process of metal solidification is affected not only by macroscopic conditions, but also by microcosmic internal characteristics. The most important factor of internal characteristic is the anisotropy phenomenon at the solid/liquid interface, and it is a key parameter affecting the evolution of crystal morphology. As long as free dendrites form stable morphology of tip, it must have anisotropy. At the same time, the growth direction and radius of dendrites tip is related to the anisotropy of interface.

Anisotropy of solid/liquid interface includes interface energy anisotropy and interface dynamics anisotropy[1]. KESSLER and LEVINE[2−5] studied the dendrite solidification process controlled by heat diffusion and concluded that the interface energy anisotropy can not only determine the dendrite tip growth speed by monotone value but also affect the dendrite morphology evolution and growth stability. SAITO et al[6] studied the dendrite growth controlled by the solute diffusion and their results showed that interface energy anisotropy inevitably existed in dendrite growth process. The interface dynamics anisotropy[3−5, 7−8] influences the dendrite interface growth speed. YOUNG et al[9] proposed that the interface dynamics could be related to the interface crystal orientation.

The simulation of the solidification microstructure evolution by phase field model has been a hot field for recent years. In the phase field model[10−15], the effect of anisotropy could be expressed by the angle function between the interfacial normal orientation and the specific orientation. At present, the investigations on phase field model are mainly focused on the plane of weak anisotropy (the coefficient of anisotropy is less than 0.067), and the investigations on the plane of strong anisotropy are very few[16−18]. Until recently, EGGLESTON[19] presented the modification method of strong anisotropy. The phase field model under interface proposed by LO and KARMA[20], ROBERT[21] has important theoretical and practical value, and it can be used to qualitatively simulate growth of dendrites. In this work, the interface energy anisotropy and interface dynamics anisotropy are introduced to describe the dendrite growth precisely. And this could actually describe the evolution of crystal structure and establish the foundation of studying the crystal growth in complex

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condition.

2 Phase field model

According to Karma's thin interface theory, phase field model of non-isothermals pure substance is constructed based on the entropy function.

Eqn.(1) is the phase field governing

$$\frac{\bar{\varepsilon}^2 W^2(\theta)}{m}\frac{\partial \Phi}{\partial t}=\frac{\partial}{\partial x}\left(|\nabla\phi|^2 W(\boldsymbol{n})\frac{\partial W(\boldsymbol{n})}{\partial(\partial_x\phi)}\right)+$$

$$\frac{\partial}{\partial y}\left(|\nabla\phi|^2 W(\boldsymbol{n})\frac{\partial W(\boldsymbol{n})}{\partial(\partial_y\phi)}\right)+\frac{\partial}{\partial z}\left(|\nabla\phi|^2 W(\boldsymbol{n})\frac{\partial W(\boldsymbol{n})}{\partial(\partial_z\phi)}\right)+$$

$$\nabla\cdot\left(W^2(\boldsymbol{n})\nabla\Phi\right)-(-\Phi+\Phi^3)-(1-2\Phi^2+\Phi^4)\psi u \qquad (1)$$

where $\boldsymbol{t}$ is non-dimensional time, $\boldsymbol{t}=t/\left(\omega^2/D\right)$; $\bar{x}$ is non-dimensional length, $\bar{x}=x/\omega$; $\bar{\varepsilon}$ is non-dimensional interface thickness, $\bar{\varepsilon}=\varepsilon/\omega$; $\bar{\tau}=\alpha\tau D/\omega^2=\bar{\varepsilon}^2/m$, and $m=\mu\delta T_{\mathrm{M}}/(DL)$ are the non-dimensional dynamics coefficient; W is the parameter related to the interface thickness. W is selected as 2.3×10^{-8} m, and the mesh dimension are selected as dx=dy=0.4, dt=0.005.

Pure nickel is selected to do the simulation, and the calculation parameters are listed in Table 1.

Table 1 Thermo-physical parameters of pure nickel

L/(J·m^{-3})	c/(J·m^{-3}·K^{-1})	σ/(J·m^{-2})
2.35×10^9	5.42×10^6	0.37
D_{T}/(m^2·s^{-1})	β/(s·m^{-1})	d_0/m
1.55×10^{-5}	0.5	0.627×10^{-9}

3 Effect of interface anisotropy on equilibrium state

In whole description of the simulation of dendrites growth, the anisotropy must be considered, which exists on the solid/liquid interface, as shown in Fig.1.

During the growth of 3D dendrites, the forms of interfacial energy and interfacial dynamics anisotropy in the phase field are as follows.

The interfacial energy anisotropy:

$$W(\boldsymbol{n})=W_0 A_S(\boldsymbol{n}) \qquad (2)$$

where $W(\boldsymbol{n})$ is the interfacial energy.

The interfacial dynamics anisotropy:

$$\tau(\boldsymbol{n})=\tau_0 A_S(\boldsymbol{n})^2 \qquad (3)$$

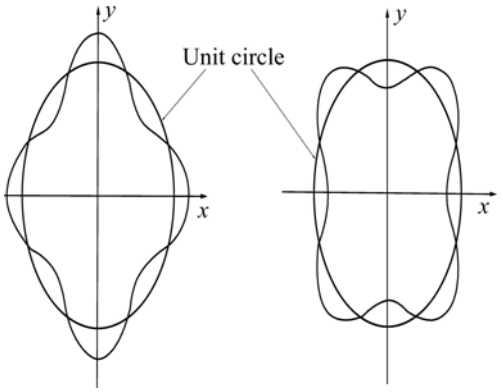

Fig.1 Expression of anisotropy

$$A_S(\boldsymbol{n})=1-3\varepsilon_4+4\varepsilon_4\frac{(\partial_x\phi)^4+(\partial_y\phi)^4+(\partial_z\phi)^4}{|\nabla\phi|^4} \qquad (4)$$

where ε_4 is the coefficient of anisotropy, $\boldsymbol{n}$ is the vector of interface normal, and it is equal to $\nabla\Phi/|\nabla\Phi|$.

Using spherical coordinates, Eqn.(4) can be expressed as

$$A_S(\boldsymbol{n})=1-3\varepsilon_4+4\varepsilon_4[\sin^4\theta(\cos^4\varphi+\sin^4\varphi)+\cos^4\theta] \qquad (5)$$

Interface anisotropy is usually expressed by using external graphs of $A_S(\boldsymbol{n})$ and $1/A_S(\boldsymbol{n})$, and $A_S(\boldsymbol{n})$ is only a function of θ in the planar space. The balanceable shapes which conform to the Wuff law correspond to the $A_S(\boldsymbol{n})$ extremal graphs, which have already been analyzed above. In the 3D space, $A_S(\boldsymbol{n})$ is the function of θ and φ, so it is difficult to analyze the lost crystal direction, and Hoffman and Cahn vector $\boldsymbol{\xi}$ is used here. The form of vector $\boldsymbol{\xi}$ is shown as follows:

$$\boldsymbol{\xi}=\gamma\boldsymbol{n}+\frac{\partial\gamma}{\partial\theta}\boldsymbol{\theta}+\frac{1}{\sin\theta}\frac{\partial\gamma}{\partial\varphi}\boldsymbol{\varphi} \qquad (6)$$

Let $\gamma(\boldsymbol{n})=A_S(\boldsymbol{n})$, $\boldsymbol{n}$, $\boldsymbol{\theta}$, $\boldsymbol{\varphi}$ is the unit vector in the spherical coordinates. To the vector $\boldsymbol{\xi}$, the Gibbs-Thomson equation which considered the anisotropy is shown as follows:

$$T=T_{\mathrm{M}}-\frac{T_{\mathrm{M}}}{L_{\mathrm{V}}}\nabla_{\mathrm{s}}\cdot\boldsymbol{\xi} \qquad (7)$$

where T_{M} is the melting point, and L_{V} is the latent heat.

The balanceable shape can be expressed as

$$\gamma(\boldsymbol{n})=\frac{2T_{\mathrm{M}}}{(T_{\mathrm{M}}-T)L_{\mathrm{V}}}\boldsymbol{\xi}(\boldsymbol{n},\boldsymbol{\theta},\boldsymbol{\varphi}) \qquad (8)$$

Eqn.(7) indicates that the balanceable shape is similar to extremal graph $\boldsymbol{\xi}$.

Figs.2−6 show the polar maps of $A_S(\boldsymbol{n})$,$1/A_S(\boldsymbol{n})$, $\boldsymbol{\xi}$ with the different anisotropy coefficient. It can be seen that when γ is less than 0.33, all of the interface growth directions is steady; and the interface is smooth and continuous. And when γ is larger than 0.33, some certain

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