Rev. Adv. Mater. Sci. 33 (2013) 246-250

SIMULATION OF DENDRITIC CRYSTAL GROWTH OF PURE Ni USING THE PHASE-FIELD MODEL

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Received: October 17, 2011

Abstract. The phase-field model is used in the numerical simulation of dendritic crystal growth in pure Ni in supercooled melt. Effect of anisotropy, undercoolings and thermal noise on the dendritic crystal growth is investigated in this paper. The simulated results indicate that with anisotropy increasing, growth rate of dendrite tip is accelerated and characteristic of dendritic structure is more obvious; As the degree of supercooling increases, stability of dendrite tip will be damaged, the dendrite tip branching-off will happen. Stirring power can promote side-branching, but does not affect growth state of dendritic crystal.

1. INTRODUCTION

Recently, numerical simulation of metal solidification has made a great progress and at the same time numerical simulation of microstructure has also made a progress. Generally, the method of numerical simulation of microstructure develops rapidly, which includes the definition method, the random method and the phase-field model. The phase field model [1-9] is based on statistic physics. According to Ginzburg-Landau phase theory, differential equation, ordering potential and thermodynamic driving force are combined. The answer of the phase-field model equation can describe the condition, shapes and movement of the solid-liquid interface. The equation of the phase-field model is coupled with others (temperature field, concentration field, velocity field), so the dendritic crystal growth in solidification can be simulated accurately.

2. PHASE FIELD MODEL

Diffusion interface model is adopted in simulation of dendritic growth when the phase-field model is used, a phase-field variable Φ is introduced, standing for physical state(liquid or solid) of the system. Phase in the phase-field system has a constant value, for example, Φ = 1 stands for the solid phase, Φ = -1 represents the liquid phase, the value of Φ varies continuously between 1 and 0 at the *S*/*L* interface. It can be seen clearly from Fig. 1 that there is a diffusion interface between *L* and *S*.

2.1. The equation of phase-field model in pure material

Equation of phase-field model can be derived from Free energy *F* or entropy *S* according to the Ginzburg-Landau theory [10], which is called free energy function model or entropy function model. Entropy function model is used in this article

$$\tau\dot{\phi} = L_0\left(\frac{1}{T_M} - \frac{1}{F}\right)p'(\phi) - \frac{W_f}{2}g'(\phi) + \frac{\varepsilon_f^2}{T}\nabla^2\phi, \quad (1)$$

$$c_v\dot{T} + L_0 p'(\phi)\dot{\phi} = k\nabla^2 T, \quad (2)$$

where τ is a phase-field parameter related to interface dynamics, ϕ is a phase-field variable, L_0 is latent heat of solidification, T_M is the solidification

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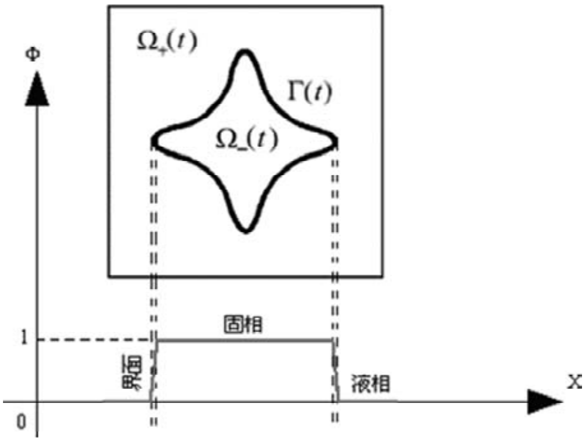

Fig. 1. Diffusion interface model.

temperature, $g(\Phi) \equiv \lambda^{-1}\partial f(\Phi,T)/\partial T\big|_{T=T_M}$ is odd function of ϕ, ε_f is a gradient correction coefficient.

2.2. Phase-field model with anisotropy factor

In the growth of 2-D dendrite, the interface energy anisotropy and interface kinetics anisotropy are introduced in the phase-field and disposed as following:

Anisotropy factor of interfacial energy:

$$W(\theta) = W_0\left(1+\gamma\cos\lambda\left(\theta-\theta_0\right)\right). \quad (3)$$

Anisotropy factor of interface kinetics:

$$\tau(\theta) = \tau\left(1+\gamma\cos\lambda\left(\theta-\theta_0\right)\right)^2. \quad (4)$$

In the equation above, W_0 is interface thickness, a_s is anisotropy factor, θ is the angle between axis direction and the perpendicularity direction, $\theta = \nabla\Phi/|\nabla\Phi|$, λ is anisotropy modulus, a general value is 4 or 6, γ is anisotropy coefficient, a general value is between 0.001~0.07, the larger the value is, the greater the anisotropy strength is, the commonly used value is between 0.02~0.05.

Anisotropy factor is introduced, the interface-analyze model proposed by Karama is used, where ϕ = 1 stands for solid phase, and ϕ = -1 stands for liquid phase. The non-dimensional phase-field model as following:

$$\frac{\bar{\varepsilon}^2 W^2(\theta)}{m}\frac{\partial\Phi}{\partial t} = -\frac{\partial}{\partial_x}\bar{\varepsilon}\left(W(\theta)W'(\theta)\frac{\partial\Phi}{\partial y}\right)+ \frac{\partial}{\partial y}\bar{\varepsilon}^2\left(W(\theta)W'(\theta)\frac{\partial\Phi}{\partial x}\right)+\bar{\varepsilon}^2\nabla\cdot\left(W^2(\theta)\nabla\Phi\right)- \left(-\Phi+\Phi^3\right)-\left(1-2\Phi^2+\Phi^4\right)\psi u, \quad (5)$$

where $u = (T - T_M)/(L/c_P)$ is a dimensionless temperature, $\vec{t} = \frac{t}{w^2/D}$ - a dimensionless time, $\bar{x} = \frac{x}{w}$ - a dimensionless length, $\bar{\varepsilon} = \frac{\varepsilon}{w}$ - dimensionless interface thickness, $\bar{\tau} = \frac{a\tau D}{w^2} = \frac{\bar{\varepsilon}^2}{m}$, $m = \frac{\mu\sigma T_M}{DL}$ is dimensionless interface kinetic coefficient, W is the parameters related interface thickness.

2.3. Phase-field with fluctuation

In order to simulate random fluctuation in the actual solidification, fluctuation should be introduced, so the phase-field equation becomes [11]:

$$\tau\dot{\phi} = L_0\left(\frac{1}{T_M}-\frac{1}{T}\right)p'(\phi)-\frac{W_f}{2}g'(\phi)+\frac{\varepsilon_f^2}{T}\nabla^2\phi+f_\phi, \quad (6)$$

$$c_v\dot{T} + L_0 p'(\phi)\dot{\phi} = k\nabla^2 T + \nabla\cdot q^{st}. \quad (7)$$

Correlation function of random item $\nabla\times q^{5t}$ and f_Φ as follows:

$$\left\langle q_u^{st}(x,t)q_v^{st}(x',t')\right\rangle = 2k_B T^2 k\delta_{uv}\delta\left(x-x'\right)\delta\left(t-t'\right), \quad (8)$$

$$\left\langle f_\phi(x,t)f_\phi(x',t')\right\rangle = 2k_B\tau\delta\left(x-x'\right)\delta\left(t-t'\right), \quad (9)$$

where k_B is the Boltzmann constant, ∇q^{5t} and f_Φ follow the Gaussin distribution.

$$F_\Phi = \frac{2k_B T_M^2 c}{L^2 l^d}\frac{W}{d_0}I,$$

$$F_u = \frac{2k_B T_M^2 c}{L^2 l^d},$$

where F_u is thermal perturbation, F_ϕ is an interface fluctuation perturbation.

2.4. Physical property parameters

Pure Ni is chosen as the research object, and the physical property parameters in the calculation are: σ = 3.70 μJcm^{-2}, T_M = 1728K, L = 2.350 KJ×cm^{-3}, c = 5.42 J×(K×cm^3)$^{-1}$, μ = 285 cm×(K×s)$^{-1}$, κ = 0.155 cm^2×s^{-1}, and the other parameters: w = 2.1 μm, α = 400, m = 500 and so on.

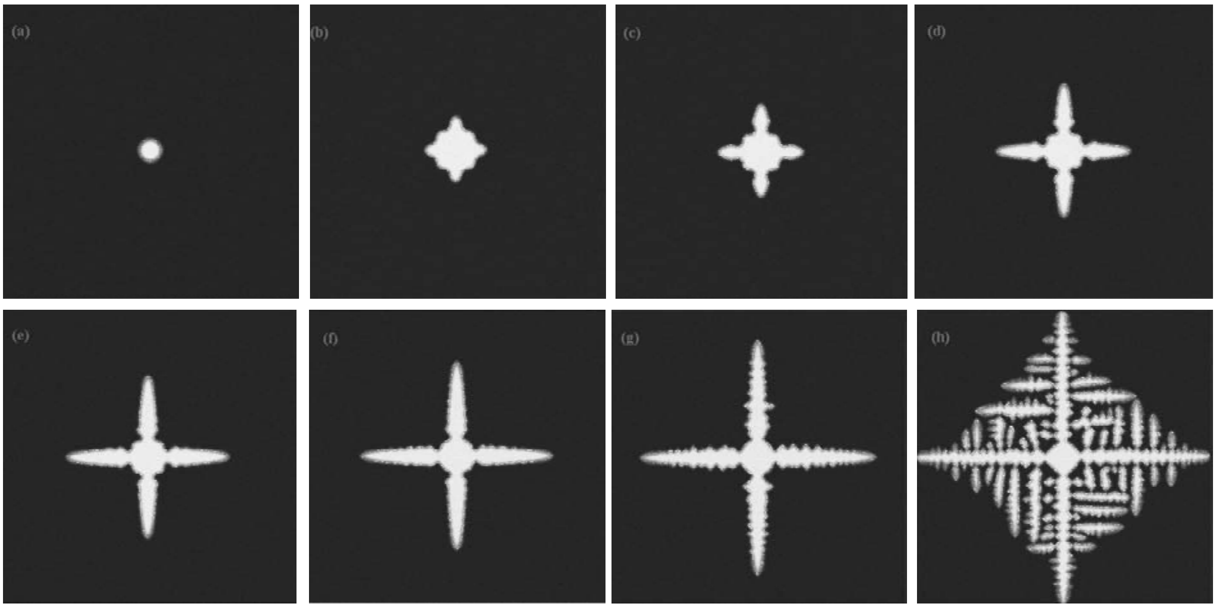

Fig. 2. Influence of anisotropy coefficient on dendrite growth. (a) $\gamma = 0$; (b) $\gamma = 0.01$; (c) $\gamma = 0.02$; (d) $\gamma = 0.03$; (e) $\gamma = 0.04$; (f) $\gamma = 0.05$; (g) $\gamma = 0.06$; (h) $\gamma = 0.0667$.

2.5. Initial condition and boundary condition

For initial nuclei radius r_0, the initial condition in the calculation is:

If $x^2 + y^2 \leq r_0^2$, $\Phi = 1$, $T=T_0$, $c = c_0$;

If $x^2 + y^2 > r_0^2$, $\Phi = -1$, $T = T_0$, $c = c_0$;

where x and y stand for coordinate axis, T_0 is initial temperature in undercooling melt, in the calculation of the regional border, Zero-Neumann boundary condition is chosen in the phase-field and temperature-field.

2.6. Numerical calculation method

The number of calculation mesh in phase-field and temperature-field is 800×800, the size is 1×10^{-8} m, the initial nucleation is assumed as a spherical whose radius is 3×10^{-8} m. In the calculation process, the radius of nuclei can be changed according to requirement. The number of nuclei should be less than or equal to the largest nucleation number. Use the second-order accurate stop-and-poor central scheme for phase field problem of numerical computation. Use the ADI algorithm for the equation for the temperature field control equation, this algorithm is between fully explicit and implicit completely, with the display format for a simple calculation, the calculation of the advantages of the twisted and implicitly consistent unconditionally.

3. SIMULATION RESULTS AND ANALYSIS

3.1. Influence of anisotropy degree on dendritic growth

Interface anisotropy coefficient γ shows the tension of interfacial surface, interface thickness and anisotropy degree of interface kinetics [12]. A small amount of thermal noise is added in this article, other parameters are kept unchanged, the value of anisotropic coefficient γ is changed sequently. The results is shown in Fig. 2 with anisotropy coefficient increased, the grain is gradually changing to equated dendrite, and the dendrite tip branching-off will not happen; at the same time, the dendrite tip becomes more and more sharp. Thus, if the anisotropy coefficient is 0 or too small, equiaxed dendrite will not come into being; under the same conditions, the larger the anisotropy coefficient is, the faster the dendrite grows. When the anisotropy coefficient value equals to 6 or more, dendrite variation will happen. The reason is that when as anisotropy coefficient increases, the thermal noise is likely to be amplified, the front interface will become unstable, the grain shape may becomes complicated.

3.2. The influence of super-cooling degree on dendrite growth

According to the principle of metal crystallization, undercooling ΔT has an important impact on

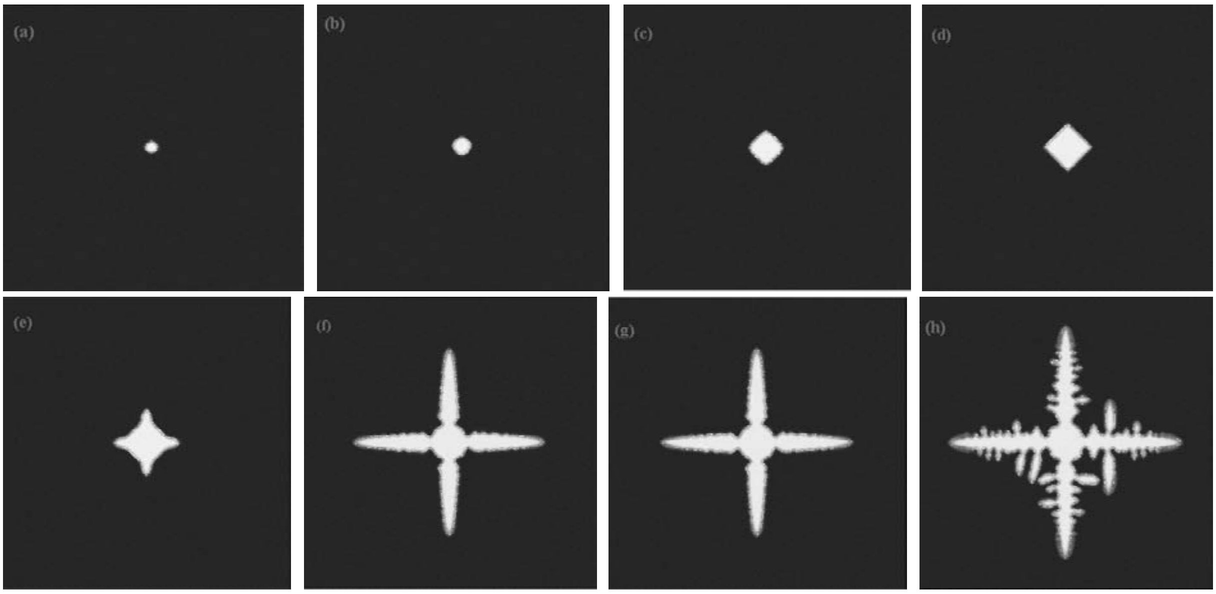

Fig. 3. The influence of undercooling on dendritic growth. (a) $\Delta T = 0$; (b) $\Delta T = 0.1$; (c) $\Delta T = 0.3$; (d) $\Delta T = 0.4$; (e) $\Delta T = 0.45$; (f) $\Delta T = 0.475$; (g) $\Delta T = 0.5$; (h) $\Delta T = 0.525$.

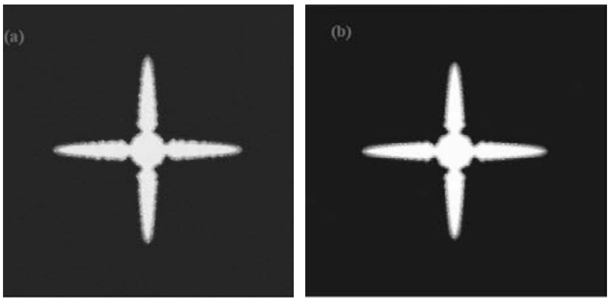

Fig. 4. Morphologies of dendritic growth simulated by phase field with and without noise. (a) Phase-field with noise; (b) phase-field without noise.

nucleation and growth processes of equiaxed grain. The same computing time and simulate regional is chosen in this paper. With other parameters unchanged, undercooling ΔT is changed continuously; the results are shown in Fig. 3. As can be seen from Fig. 3, the dendrite does not grow any more when ΔT changes from 0 to 0.3, It can be known that the smaller ΔT is, the more difficultly the dendrite grows. As the value of ΔT increases, the dendrite trunk becomes thinner, meantime the dendrite tip radius decreases, the growth rate increases. With ΔT increase, the dendrite trunk becomes instability, dendrite side-branching become more and more active, when ΔT is greater than 0.5, the dendrite tip branching-off can be seen, the side-branching are also extremely active, when the undercooling degree is greater than 0.5, the dendrite tip branching-off will happen, the other branches become extremely active, branches grow more and more fast, it can be seen that the branches stretch into the undercooled melt rapidly. Under certain condition, the dendrite tip branching-off will happen.

3.3. The influence of thermal noise on the morphology of dendrite

In Fig. 4, when fluctuation is introduced, fold can be seen on the grain. Under the two conditions that fluctuation is added and not added, crystal dendrite shape is very similar, that is, the curvature radiuses of dendrite tip are very similar under the case. However, the primary branches with fluctuation are longer than that without fluctuation. That is, it grows faster than that without fluctuation, which indicates that fluctuation will promote dendrite growth.

4. CONCLUSIONS

(1) As the anisotropy coefficient increases, the dendrite gradually changes into equiaxed shape,and the trunk no longer bifurcates. At the same time, the tip of dendrite becomes more and more sharp, which

can show growth of dendrite accurately, when the anisotropy coefficient changes from 0.03 to 0.05.
(2) Low undercooling melt, growth of lateral branch is inhibited, smooth dendrites morphology can be seen; and at deep undercooling condition, the side-branches develop highly.
(3) With the same parameters, without fluctuation, the grain grows along the backbone, it is smooth and secondary arms will not appear; with fluctuation added, a little fold can be seen on the grain, the grain with grain grows faster than that without fluctuation, indicating that fluctuation can promote dendrite growth.

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