In the circumstance of solidification of material at the undercooling state, there is a model called phase field model which could simulate this process well. Phase field model replace the sharp interface by a smooth and continuous interface of very small width, so parameters in the model can be calculated by a certain set of equation, and the simulation result fits the reality better.

This diffusion layer is given by the phase field parameter φ, which is a function of space and time. The phase field parameter ranges from 0 to 1, φ=0 represents for liquid, and φ=1 represents for solid. This phase field parameter distinguishes the solid phase from the liquid phase and the transition layer in between.

In this model, there are two basic function controls the phase and temperature.

1. The function of phase.

The basic equation controls the phase with time is as 1.1. It gives us the relationship between the free energy of the transition layer and its front tracking. It is the basic phase-field equation which gives us the location and velocity of interface.

$$\frac{\partial \varphi}{\partial t} = -M \frac{\delta F}{\delta \varphi} \tag{1.1}$$

M represents for the motivation speed of phase field, it depends on components of material, for different kinds of material, it is set of different constants.

F is a free energy function of Ginzburg-Landau, it could be explained as 1.2. F is a function that accounts for the mixing of energy in the interface due to the evacuation of heat and it describes the solid and liquid phases.

$$F = \int [\frac{\varepsilon^2}{2} |\nabla \varphi|^2 + f(\varphi, c, T)] dV \tag{1.2}$$

In 1.2, ε is interfacial width and f represents for density of free energy.

The partial function of F over φ can be written as 1.3.

$$\frac{\delta F}{\delta \varphi} = -\nabla \left[\frac{\partial F_v}{\partial (\nabla \Phi)} \right] + \frac{\partial F_v}{\partial \varphi} \tag{1.3}$$

As the equation in 1.4, we can calculate the partial equation as 1.5.

$$F_v = \frac{\varepsilon^2}{2} |\nabla \varphi|^2 + f(\varphi, c, T) \tag{1.4}$$

$$\frac{\partial \varphi}{\partial t} = M [\varepsilon^2 \nabla^2 \varphi - f_\varphi] \tag{1.5}$$

For the general model, we write f as the combination of sum of solid free energy, liquid free energy and residual free energy.

$$f = h(\varphi) f^S + (1 - h(\varphi)) f^L + W g(\varphi) \tag{1.6}$$

In this model, we used the double well free energy functional with prescribed value as:

$$f(\varphi, m) = \frac{1}{4}\varphi^4 - \left(\frac{1}{2} - \frac{1}{3}m\right)\varphi^3 + \left(\frac{1}{4} - \frac{1}{2}m\right)\varphi^2 \tag{1.7}$$

This double well free energy functional also ensures the growth of the solid phase at the expense of liquid phase. When the free energy of the liquid phase decreases then the liquid phase transforms into solid phase.

After calculation the partial for f of φ is as 1.8.

$$f_\varphi = -\varphi(1 - \varphi)\left(\varphi - \frac{1}{2} + m\right) \tag{1.8}$$

The partial equation can be written as 1.9

$$\tau\frac{\partial\varphi}{\partial t} = \varphi(1 - \varphi)\left(\varphi - \frac{1}{2} + m\right) + \nabla \cdot \left(\varepsilon^2 \nabla \phi\right) - \nabla \cdot \left(|\nabla\varphi|^2\varepsilon\frac{\partial\varepsilon(\vec{v})}{\partial\vec{v}}\right) \tag{1.9}$$

τ is equals to 1/M, physical meaning is the relaxation time, is a constant.

In 1.7, m is a dimensionless temperature. In this model we calculate m as 1.10. It is an experimental result, in this relation the modification result will be more accurate.

$$m = \frac{\alpha}{\pi}\arctan[\gamma(T_e - T)] \tag{1.10}$$

In order to introduce anisotropy in phase field model of solidification, we assumed the interfacial width ε as a function of angle, where θ is the angle between the x -axis and ∇φ. In this model, we used 1.11 to describe the relation between them.

$$\varepsilon = \varepsilon_0(1 + \delta\cos[j(\theta - \theta_0)]) \tag{1.11}$$

And 1.12 is the definition of angle.

$$\theta = \arctan\left(\frac{\varphi_y}{\varphi_x}\right) \tag{1.12}$$

In cartesian coordinate system, the phase field model could be written as:

$$\tau\frac{\partial\varphi}{\partial t} = \varphi(1 - \varphi)\left(\varphi - \frac{1}{2} + m\right) + \nabla(\varepsilon^2)\nabla\phi + \varepsilon^2\nabla^2\varphi - \frac{\partial}{\partial x}\left(\varepsilon\varepsilon'\frac{\partial\varphi}{\partial y}\right) + \frac{\partial}{\partial y}\left(\varepsilon\varepsilon'\frac{\partial\varphi}{\partial x}\right) \tag{1.13}$$

And 1.13 is the equation for simulation calculation.

2. The function of time

Another basic function for controlling temperature is as 2.1:

$$\frac{\partial T}{\partial t} = \nabla^2 T + K\frac{\partial\varphi}{\partial t} \tag{2.1}$$

It is derived from the conservation law of enthalpy. T is non-dimensionalized so that the characteristic cooling temperature is 0 and the equilibrium temperature is 1. K is a dimensionless latent heat which is proportional to the latent heat and inversely proportional to the strength of the cooling.

The following simulation is based on equation 1.13 and 2.1.