A Phase Field Method Based Model for Solidification

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The phase field method is a technique for modeling evolution of a system under a thermodynamic driving force. The system is described in terms of an order parameter. Examples of order parameter include temperature, phase fraction, magnetization etc. Since we want to model solidification, we will choose the order parameter, φ to be the crystallographic disorder. In this case, the solid state corresponds to φ = 0 and the liquid state corresponds to φ = 1. Next we develop an expression for the total bulk free energy (g) of the system.

$$g = \left(\frac{T_m - T}{T_m}\right)(hg_S + (1-h)g_L) + Qf \tag{1}$$

$$h = \phi^2(3 - 2\phi) \tag{2}$$

$$f = \phi^2(1-\phi)^2 \tag{3}$$

Here g_L and g_S are the free energy of the pure solid and pure liquid state. Q is the activation barrier. The phase field method models a diffuse interface. Hence the total free energy of the system is given as the sum of the bulk term and the gradient term. The gradient term is equivalent of interface energy.

$$g_{PF} = k(\nabla\phi)^2 + g \tag{4}$$

The evolution of the order parameter is described as

$$\frac{d\phi}{dt} = -M\frac{dg}{d\phi} \tag{5}$$

With the form of the bulk free energy assumed above, this gives us

$$\frac{d\phi}{dt} = M[k\nabla^2\phi + \left(\frac{T_m - T}{T_m}\right)(h'(g_L - g_S) + Qf'] \tag{6}$$