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A SEMI-SHARP PHASE FIELD METHOD FOR QUANTITATIVE PHASE CHANGE SIMULATIONS

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Summary The standard phase field model for simulation of phase change requires an asymptotic analysis in a vanishing interface width, in order to connect the model parameters to the sharp interface parameters, which has hampered the quantitative usefulness of the method. In this talk a modification of the method is presented, that allows the sharp and phase field parameters to be identified, in principle without restrictions on the model parameters.

INTRODUCTION

The phase-field method [1, 2, 3] has become very popular for simulations of the evolution of microstructures in solidification and other phase change problems, such as dendritic growth of crystals in an undercooled melt. The governing equations are derived from the thermodynamic potentials of the system, together with the assumption of a surface energy associated with a diffuse solid/liquid interface. It is thus possible to consider different physical situations with relative ease, such as grain boundaries, mixtures, etc. The phase is represented by introducing a scalar variable that has different constant values in the solid and liquid, and a steep transition between the two in the diffuse interface.

The problem with the method is that in its original form, the width of the diffuse interface must be prohibitively small for the results to match the proper interface kinetics, [4, 5], typically $W^* << d_0^*$, where W^* is the interface width, and $d_0^* = cT_m\gamma/L^2$ is the capillary length, which in typical cases can be in the order of nanometers (c is specific heat, T_m temperature of a flat interface at equilibrium, γ surface energy, and L latent heat). As a remedy to this, Karma and Rappel [6, 7], introduced the thin interface version of the method, whereby the asymptotic analysis of the phase field equations is taken to second order in interface width, allowing the kinetics to be identified under less stringent conditions [6, 7]. Also, in the thin interface limit the kinetic term can be eliminated from the undercooling, if that is desired. However, the seemingly modest extension of this analysis to nonhomogeneous properties, such as different diffusion coefficients in the solid and liquid, requires nontrivial modifications of the model equations, [8, 9].

In this talk the standard phase field method is simplified to the point that a relevant reduced problem can be solved analytically. Contact can thus be made between the phase field and the sharp interface descriptions, in principle without restrictions on the model parameters, other than the inevitable condition that the interface width is small compared to local radius of curvature.

MATHEMATICAL MODEL

For clarity we will describe the model for the simple situation of thermal solidification of a pure material with isotropic Gibbs-Thomson kinetics at the interface,

$$-\theta_i = \frac{V}{\mu} + \frac{d_0}{R} \tag{1}$$

Here V denotes the normal speed of the interface, μ the kinetic coefficient, R the local radius of curvature, and d_0 the capillary length. Here, and in the following, we have nondimensionalized temperature according to $\theta = c(T - T_m)/L$, lengths with an (arbitrary) reference length H, time with H^2/κ, where κ is the heat diffusivity.

As a starting point, the phase field model is written as

$$\tau\frac{\partial\phi}{\partial t} = W^2\nabla^2\phi - f'(\phi) - g'_\delta(\phi)\cdot h(\lambda\theta) \tag{2}$$

Here ϕ is the phase field variable which is $+1$ in the solid and -1 in the liquid. W denotes the interface width parameter, τ will be linked to the kinetic undercooling, and λ to the capillary length.

The conservation of heat takes the form:

$$\frac{\partial\theta}{\partial t} = \nabla^2\theta + \frac{\partial g_\delta(\phi)}{\partial t} \tag{3}$$

The function $f(\phi)$ should be a double well, with minima at $\phi = \pm 1$, $g_\delta(\phi)$ accounts for the change in internal energy on phase change and should increase from 0 to 1 as ϕ goes from -1 to $+1$. A standard choice is $f(\phi) = (1-\phi)^2(1+\phi)^2$ and $g_\delta(\phi) = 15/16(\phi^5/5 - 2\phi^3/3 + \phi) + 1/2$. We note that the two functions $f(\phi)$ and $g_\delta(\phi)$ are independent, and that there is a considerable degree of freedom in choosing these. Here we have also introduced a function $h(\lambda\theta)$ in the last term of equation (2), which in the standard model is $h(\lambda\theta) = \lambda\theta$.

We now introduce the following modifications:

i) The function $g_\delta(\phi)$ is chosen as a smoothed step function, $g_\delta(\phi) = (1 + \phi\sqrt{(1+\delta^2)/(\phi^2+\delta^2)})/2$, that jumps from 0 to 1 over an interval of width $\sim\delta$ at $\phi = 0$. The model we are interested in is then obtained in the limit $\delta = 0$.

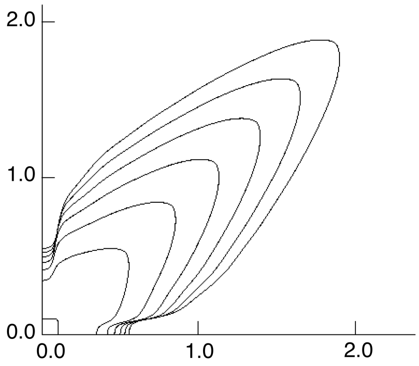

Figure 1. Sequence of interfaces for a developing needle crystal, $t = 0, 0.1, ..., 0.6$. The total size of the domain is 10 x 10.

ii) In order to evaluate the kinetics of the model exactly, we choose a simpler form of $f(\phi)$, i.e $f(\phi) = (\phi - 1)^2$ for $\phi > 0$, and $f(\phi) = (\phi + 1)^2$ for $\phi < 0$.
iii) With these choices of $f(\phi)$ and $g_\delta(\phi)$, an explicit function $h(\lambda\theta_i) = \frac{1}{2}\lambda\theta_i\sqrt{8 + (\lambda\theta_i)^2}$, will give linear Gibbs-Thomson kinetics, also for large values of $\lambda\theta$.
We will view the interface as being given by the contour generated by $\phi = 0$, i.e. the interface is 'sharp' in this sense. With the choices in i)-iii), a reduced problem can be formulated, see [10], assuming a profile of ϕ that is translating with a quasi-constant shape, in the presence of mild curvature, i.e. $R >> W$. This can be solved exactly to yield a relation between interface temperature, curvature and speed at the position where $\phi = 0$. By comparing with Gibbs-Thomson kinetics, eq (1), we can now identify the phase field and the sharp interface parameters as $\mu = W\lambda/\tau$, $d_0 = W/\lambda$.

SAMPLE COMPUTATION

To illustrate the practical use of the method, we simulated a typical case of solidification with an undercooling of 0.5, i.e. $\theta_\infty = -0.5$, and the sharp interface parameters $\mu = 117.5$ and $d_0 = 0.001191$. We also included anisotropy by letting the surface energy vary by a factor $(1 + \epsilon cos(4\beta))$, with β being the angle between an interface normal and the preferred growth direction. The value of the anisotropy parameter was $\epsilon = 0.04$. The phase field parameters λ and τ are determined from μ and d_0 and a desired width of the transition region, here $W = 0.02$, which gives $\lambda = 16.792$ and $\tau = 0.002858$. This case was deliberately chosen with a quite thick interface, i.e., λ considerably larger than unity. Figure 1 shows the interface obtained with $W = 0.02$ as it develops for times from 0 to 0.6. The shape evolves into a typical needle crystal, where the tip attains a nearly parabolic shape and a constant speed. A direct comparison of the temperature obtained at the interface and that predicted from equation (1) shows a very good agreement. This computation was made using adaptive finite elements implemented using our toolbox femLego [11]. In the talk additional examples and applications will be presented as time and results allow.

CONCLUSION

In summary, we have presented a few simple modifications of the standard phase field model that will allow the correct kinetics to be simulated with quite thick interfaces. The only restrictions are in terms of numerical resolution, and that radii of curvature should be larger than interface widths. The model presented retains its connection to the thermodynamic derivation of phase fields, giving hope that it can be applied to many different situations. The presented method can perhaps also be viewed as an intermediate between diffuse interface phase-field formulations and proper sharp interface or level set methods.

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