PRISMS-PF Application Formulation: alloySolidification_uniformT

This example application implements a simple model to simulate solidification of a binary alloy A-B in the dilute limit with component B acting as a solute in a matrix of A. The implemented model was introduced by Karma. [1] in 2001. In this model, latent heat is assumed to diffuse much faster than impurities and, therefore, the temperature field is considered to be fixed by external conditions. In contrast to *alloySolidification*, this application considers solidification under uniform temperature. In the default settings of the application, the simulation starts with a circular solid in the corner of a square system. The evolution of the system is calculated for a supersaturation value, Ω, that remains constant throughout the simulation. As this seed grows, three variables are tracked, an order parameter, ϕ, that denotes whether the material a liquid ($\phi = -1$) or solid ($\phi = 1$), the solute concentration, c, and an auxiliary term, ξ.

1 Model

Pending: Deriving the following equations from the free energy

The coupled governing equations for the ϕ and c are

$$\tau(\theta)\frac{\partial \phi}{\partial t} = \xi(\phi, c), \tag{1}$$

where

$$\xi(\phi, c) = -f'(\phi) - \frac{\lambda}{1-k} g'(\phi)(e^u - 1) + \nabla \cdot [W(\theta)^2 \nabla \phi] - \frac{\partial}{\partial x}\left[W(\theta)W'(\theta)\frac{\partial \phi}{\partial y}\right] + \frac{\partial}{\partial y}\left[W(\theta)W'(\theta)\frac{\partial \phi}{\partial x}\right] \tag{2}$$

and

$$\frac{\partial c}{\partial t} = \nabla \cdot \vec{j}, \tag{3}$$

where

$$\vec{j} = -Dcq(\phi)\nabla(u) - aWc_l^0(1-k)e^u \frac{\partial \phi}{\partial t}\frac{\nabla \phi}{|\nabla \phi|} \tag{4}$$

Pending: defining u, θ, $W(\theta)$, and the other variables and constants

2 Model Constants

Pending: Update this section

ϵ: Strength of the anisotropay (ϵ_4 for a solid with fourfold anisotropy)
k: Partition coefficient
c_0: Initial liquid concentration (c_∞)
λ: Coupling constant (setting this value fixes the interface width)
$\tilde{D}$: Dimensionless solute diffusivity in the liquid phase.
$\tilde{V}_p$: Dimensionless steady-state velocity of the tip.
$\tilde{l}_T$: Dimensionless thermal length.
U_0: Initial constitutional undercooling of the system ($U_0 = -1$ sets the concentration of the liquid as c_∞

and of the solid as kc_∞)
U_{off}: Undercooling offset that determines the initial temperature at the interface ($U_{\text{off}} = 0$ sets it to the solidus temperature, $U_{\text{off}} = 1$ sets it to the liquidus temperature).
$\tilde{y}_0$: Initial solid-liquid interface position relative to the bottom of the system ($\tilde{y} = 0$)

3 Time Discretization

Considering forward Euler explicit time stepping, we have the time discretized kinetics equations:

$$\phi^{n+1} = \phi^n + \frac{\xi^n}{\tau^n}\Delta t, \tag{5}$$

$$c^{n+1} = c^n + \Delta t \left\{ Dc^n q(\phi^n)\nabla(u^n) + aWc_l^0(1-k)(e^u)^n \left(\frac{\partial \phi}{\partial t}\right)^n \frac{\nabla\phi^n}{|\nabla\phi^n|} \right\} \tag{6}$$

and

$$\begin{aligned} \xi(\phi, c) = &- f'(\phi^n) - \frac{\lambda}{1-k} g'(\phi^n)[(e^u)^n - 1] \\ &+ \nabla \cdot [W(\theta^n)^2 \nabla\phi^n] - \frac{\partial}{\partial x}\left[W(\theta^n)W'(\theta^n)\frac{\partial \phi^n}{\partial y}\right] + \frac{\partial}{\partial y}\left[W(\theta^n)W'(\theta^n)\frac{\partial \phi^n}{\partial x}\right]. \end{aligned} \tag{7}$$

4 Weak Formulation

The weak form of the time-discretized equations for ϕ, c, and, ξ is

$$\int_\Omega \omega\phi^{n+1}\, dV = \int_\Omega \omega \underbrace{\left(\phi^n + \frac{\xi^n}{\tau(\theta^n)}\Delta t\right)}_{r_\phi} dV, \tag{8}$$

$$\begin{aligned} \int_\Omega \omega c^{n+1}\, dV = &\int_\Omega \omega \underbrace{c^n}_{r_c}\, dV \\ &+ \int_\Omega \nabla\omega \cdot \underbrace{\left[-\Delta t D\left(q(\phi^n)\nabla c^n + \frac{(1-k)q(\phi^n)c^n\nabla(\phi^n)}{1+k-(1-k)\phi^n}\right) - \Delta t a W c_l^0(1-k)(e^u)^n\left(\frac{\partial\phi}{\partial t}\right)^n \frac{\nabla\phi^n}{|\nabla\phi^n|}\right]}_{r_c x} dV, \end{aligned} \tag{9}$$

and

$$\int_\Omega \omega \xi^{n+1}\, dV = \int_\Omega \omega r_\xi\, dV + \int_\Omega \nabla \omega r_{\xi x}\, dV \tag{10}$$

where

$$r_\xi = -f'(\phi^n) - \frac{\lambda}{1-k} g'(\phi^n)[(e^u)^n - 1] \tag{11}$$

and

$$\begin{aligned} r_{\xi x} = &- \left[W(\theta^n)^2 \frac{\partial \phi^n}{\partial x} - W(\theta^n) W'(\theta^n) \frac{\partial \phi^n}{\partial y} \right] \hat{x} \\ &- \left[W(\theta^n)^2 \frac{\partial \phi^n}{\partial y} + W(\theta^n) W'(\theta^n) \frac{\partial \phi^n}{\partial x} \right] \hat{y} \end{aligned} \tag{12}$$

References

[1] A. Karma, Quantitative phase-field model of alloy solidification, *Phys. Rev. Lett.* **87**, 115701 (2001).