

# PRISMS-PF Application Formulation: alloySolidification\_uniform

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 and no diffusion in the solid. 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 an initial scaled supersaturation value,  $\Omega$ . As this seed grows, three variables are tracked, an order parameter,  $\phi$ , that denotes whether the material is a liquid ( $\phi = -1$ ) or solid ( $\phi = 1$ ), the solute concentration,  $c$ , and an auxiliary term,  $\xi$ .

## 1 Model

The free energy of the system can be written as the functional [2]

$$\mathcal{F}[\phi, c, T] = \int_{\Omega} \left[ \frac{\sigma}{2} |\nabla \phi|^2 + H f(\phi, T_M) + f_{AB}(\phi, c, T) \right] dV, \quad (1)$$

where  $\sigma$  is penalty coefficient for phase gradients. The term  $f(\phi, T_M)$  is a symmetric double-well term evaluated at the melting temperature of the pure material A,  $T_M$ . The constant  $H$  is the height of the well and  $f_{AB}(\phi, c, T)$  accounts for the relative stability of the liquid and solid phases at different temperatures, according to the phase diagram. The double-well term has the standard form given by

$$f(\phi, T_M) = -\phi^2/2 + \phi^4/4. \quad (2)$$

For a dilute binary alloy,  $f_{AB}$  can be written as

$$f_{AB}(\phi, c, T) = f^A(T_M) - (T - T_M)s(\phi) + \frac{RT_M}{v_o}(c \ln c - c) + \epsilon(\phi)c, \quad (3)$$

where  $f^A(T_M)$  is the free energy density of pure A at its melting point,  $v_o$  is the molar volume of A and  $R$  is the gas constant. The functions  $s(\phi)$  and  $\epsilon(\phi)$  are interpolation functions for the entropy and internal energy of the solid and liquid phases, respectively. The general form of the coupled governing equations for the  $\phi$  and  $c$  is

$$\frac{\partial \phi}{\partial t} = -K_{\phi} \frac{\delta \mathcal{F}}{\delta \phi} \quad (4)$$

and

$$\frac{\partial c}{\partial t} = \nabla \cdot \left( M(\phi, c) \frac{\delta \mathcal{F}}{\delta c} - \vec{j}_{at} \right), \quad (5)$$

where  $K_{\phi}$  is a kinetic constant,  $M(\phi, c)$  is the mobility of solute atoms and  $\vec{j}_{at}$  is a nonvariational anti-trapping solute current required to correct for spurious effects that arise from considering an interface thickness much larger than the physical solid-liquid interface. In the dilute limit, the solidus and liquidus lines of the  $T$  vs  $c$  phase diagram are defined by the equations

$$T_l = T_M - |m|c_l \quad (6)$$

and

$$T_s = T_M - \frac{|m|}{k} c_s, \quad (7)$$

where  $m$  is the liquidus slope and  $k = c_s/c_l$  is the partition coefficient, which relates the equilibrium concentrations,  $c_l$  and  $c_s$ , of the liquid and solid, respectively.

Considering solidification at a temperature  $T_0 < T_M$ , we define  $c_l^0 = c(T_0)$  as the equilibrium liquid concentration and  $kc_l^0$  as the equilibrium solid concentration. After nondimensionalization, the coupled governing equations for the  $\phi$  and  $c$  can be written as [1]

$$\tau \frac{\partial \phi}{\partial t} = \xi(\phi, c), \quad (8)$$

where

$$\xi(\phi, c) = -\frac{\partial f}{\partial \phi} - \frac{\lambda}{1-k} g'(\phi)(e^u - 1) + W^2 \nabla^2 \phi \quad (9)$$

and

$$\frac{\partial c}{\partial t} = \nabla \cdot \vec{j}, \quad (10)$$

where

$$\vec{j} = -Dcq(\phi)\nabla u - aWc_l^0(1-k)e^u \frac{\partial \phi}{\partial t} \frac{\nabla \phi}{|\nabla \phi|}, \quad (11)$$

and

$$u(c, \phi) = \ln \left( \frac{2c/c_l^0}{1+k-(1-k)h(\phi)} \right). \quad (12)$$

The constant  $\lambda$  is defined as  $\lambda = a_1 W/d_0$ , where  $d_0$  is the microscopic capillary length. The constants  $W$  and  $\tau$  are the unit length and time, respectively and  $D$  is the diffusivity in the liquid. The value of  $D$  is set to  $D = a_2 W^2 \lambda / \tau$  so that interface kinetics are eliminated from the velocity-dependent Gibbs-Thompson condition. The values of  $a$ ,  $a_1$ ,  $a_2$  are given in Section 2. The functions  $g'(\phi)$ ,  $h(\phi)$  and  $q(\phi)$  are given by

$$g'(\phi) = (1 - \phi^2)^2, \quad (13)$$

$$q(\phi) = \frac{1 - \phi}{1 + k - (1 - k)h(\phi)}, \quad (14)$$

and

$$h(\phi) = \phi. \quad (15)$$

Crystalline anisotropy is introduced by generalizing Eqs. (8) and (9) to

$$\tau(\theta) \frac{\partial \phi}{\partial t} = \xi(\phi, c), \quad (16)$$

where

$$\xi(\phi, c) = -f'(\phi) - \frac{\lambda}{1-k} g'(\phi)(e^u - 1) + \nabla \cdot [W(\theta)^2 \nabla \phi] - \frac{\partial}{\partial x} \left[ W(\theta) W'(\theta) \frac{\partial \phi}{\partial y} \right] + \frac{\partial}{\partial y} \left[ W(\theta) W'(\theta) \frac{\partial \phi}{\partial x} \right], \quad (17)$$

where  $\theta$  is the angle between the outward normal of the solid-liquid interface and the positive  $x$  axis. The constants  $W$  and  $\tau$  now depend on this angle and are given by  $W(\theta) = W a_s(\theta)$  and  $\tau(\theta) = \tau a_s(\theta)^2$ , respectively, where  $a_s(\theta) = 1 + \epsilon_4 \cos(4\theta)$ .

The initial condition is set by placing a solid seed in an undercooled system with a uniform scaled supersaturation value,  $\Omega = (c_l^0 - c_\infty)/[c_l^0(1-k)]$ .

## 2 Model Constants

Symbol	Value	Description
$c_l^0$	1	Reference concentration (equilibrium liquid concentration at $T_0$ )
$k$	0.15	Partition coefficient
$W$	1	Unit length
$\tau$	1	Unit time
$d_0/W$	0.277	Microscopic capillary length (with respect to W)
$a$	$1/(2\sqrt{2})$	Antitrapping term constant
$a_1$	0.8839	Coefficient $a_1$
$a_2$	0.6267	Coefficient $a_2$
$\lambda$	$a_1 W/d_0$	Parameter $\lambda$
$D$	$a_2 \lambda W^2/\tau$	Solute diffusivity in the liquid
$\epsilon_4$	0.02	Anisotropy strength
$\Omega$	0.55	Scaled supersaturation

## 3 Time Discretization

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

$$\phi^{n+1} = \phi^n + \frac{\xi^n}{\tau^n} \Delta t, \quad (18)$$

$$c^{n+1} = c^n + \Delta t \left\{ D c^n q(\phi^n) \nabla(u^n) + a W c_l^0 (1-k) (e^u)^n \left( \frac{\partial \phi}{\partial t} \right)^n \frac{\nabla \phi^n}{|\nabla \phi^n|} \right\} \quad (19)$$

and

$$\begin{aligned} \xi(\phi, c) = & -f'(\phi^n) - \frac{\lambda}{1-k} g'(\phi^n) [(e^u)^n - 1] \\ & + \nabla \cdot [W(\theta^n)^2 \nabla \phi^n] - \frac{\partial}{\partial x} \left[ W(\theta^n) W'(\theta^n) \frac{\partial \phi^n}{\partial y} \right] + \frac{\partial}{\partial y} \left[ W(\theta^n) W'(\theta^n) \frac{\partial \phi^n}{\partial x} \right]. \end{aligned} \quad (20)$$

## 4 Weak Formulation

The weak form of the time-discretized equations for  $\phi$ ,  $c$ , and,  $\xi$  is

$$\int_{\Omega} \omega \phi^{n+1} dV = \int_{\Omega} \omega \underbrace{\left( \phi^n + \frac{\xi^n}{\tau(\theta^n)} \Delta t \right)}_{r_{\phi}} dV, \quad (21)$$

$$\begin{aligned} \int_{\Omega} \omega c^{n+1} dV = & \int_{\Omega} \omega \underbrace{c^n}_{r_c} dV \\ & + \int_{\Omega} \nabla \omega \cdot \underbrace{\left[ -\Delta t D \left( q(\phi^n) \nabla c^n + \frac{(1-k)q(\phi^n)c^n \nabla(\phi^n)}{1+k-(1-k)\phi^n} \right) - \Delta t a W c_l^0 (1-k) (e^u)^n \left( \frac{\partial \phi}{\partial t} \right)^n \frac{\nabla \phi^n}{|\nabla \phi^n|} \right]}_{r_{cx}} dV, \end{aligned} \quad (22)$$

and

$$\int_{\Omega} \omega \xi^{n+1} dV = \int_{\Omega} \omega r_{\xi} dV + \int_{\Omega} \nabla \omega r_{\xi x} dV \quad (23)$$

where

$$r_{\xi} = -f'(\phi^n) - \frac{\lambda}{1-k} g'(\phi^n) [(e^u)^n - 1] \quad (24)$$

and

$$\begin{aligned} r_{\xi x} = & - \left[ W(\theta^n)^2 \frac{\partial \phi^n}{\partial x} - W(\theta^n) W'(\theta^n) \frac{\partial \phi^n}{\partial y} \right] \hat{x} \\ & - \left[ W(\theta^n)^2 \frac{\partial \phi^n}{\partial y} + W(\theta^n) W'(\theta^n) \frac{\partial \phi^n}{\partial x} \right] \hat{y} \end{aligned} \quad (25)$$

## References

- [1] A. Karma, Phase-Field Formulation for Quantitative Modeling of Alloy Solidification, *Phys. Rev. Lett.* **87**, 115701 (2001).
- [2] B. Echabbaria, R. Folch, A. Karma, and M. Plapp, Quantitative phase-field model of alloy solidification, *Phys. Rev. E* **70**, 061904 (2004).