

# Thermodynamic principles for phase-field modeling of alloy solidification

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Phase-field modeling is not only a powerful simulation tool to predict the microstructure evolution but also a useful theoretical method to study the interface kinetics. In this paper, the thermodynamic principles for and the recent progress in the phase-field modeling of isothermal solidification of binary alloys are reviewed. Different phase-field models with or without the condition of equal concentrations or equal diffusion potentials are reformulated from the entropy/free energy functional or the thermodynamic extremal principle. Their physics behind, problems and relation to the sharp interface models are analyzed. The importance to solve directly the additional constraints in the modeling system self-consistently in thermodynamics is highlighted.

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## Introduction

### Sharp interface models versus phase-field models

Many inhomogeneous systems consist of domains of well-defined phases separated by a distinct interface [1], for example the solid (*S*) and liquid (*L*) are separated by an *S/L* interface upon solidification. In the conventional sharp interface models, the interface is assumed to be infinitely sharp and for each domain, diffusional equations, conservation laws at and kinetics of the moving interface are formulated [2]. Taking the isothermal solidification of a binary alloy system as an example, the diffusion equations for solute concentration  $c_i$  ( $i = S, L$ )

$$\frac{\partial c_i}{\partial t} = -D_i \nabla^2 c_i \quad (1)$$

should be solved together with the mass conservation law at the interface

$$V(c_S^* - c_L^*) = V_m(J_B^{S*} - J_B^{L*}) = -D_S \nabla c_S^* + D_L \nabla c_L^* \quad (2)$$

and the kinetics of interface [3]<sup>1</sup>

$$\frac{V}{V_0} = -\frac{c_L^* \Delta \mu_B^* + (1 - c_L^*) \Delta \mu_A^*}{RT} \quad (3)$$

$$\frac{V}{V_{DI}} \frac{c_L^* - c_S^*}{c_S^*(1 - c_L^*)} = -\frac{\tilde{\mu}_L^* - \tilde{\mu}_S^*}{RT} = -\frac{\Delta \mu_A^* - \Delta \mu_B^*}{RT} \quad (4)$$

In the bulk phases, there is one dissipative process (i.e. solute diffusion  $J_B^i = -D_i \nabla c_i$ ). While at the interface, there are two dissipative processes (i.e. interface migration  $J_C = V/V_m$  and trans-interface diffusion  $J_D = V(c_L^* - c_S^*)/V_m$  [4]). Their dissipations  $\Delta g_C^* = c_L^* \Delta \mu_B^* + (1 - c_L^*) \Delta \mu_A^*$  is shown in the molar Gibbs free energy diagram [Figure 1](#).

Application of sharp interface models however is not predominant. First, their simulations require tracking explicitly the moving interface, which is quite difficult for the complex interface morphologies (i.e. the front-tracking problem). Second, a set of non-linear equations for interface kinetics (e.g. Eqs. (3) and (4)) must be solved at each point of the interface to obtain the interface conditions (e.g.  $c_S^*$ ,  $c_L^*$  and  $T$  for given  $V$ ) which also decreases considerably the numerical efficiency.

The above problems are avoided by the phase-field models (PFMs). By introducing the phase-field variables that are constant in each domain (e.g.  $\phi_S = \phi = 1$ ,  $\phi_L = 0$ ) and change continuously across the diffusive interface (e.g. from 1 to 0), the interface morphologies are given implicitly by the contour of constant values of phase-field variables. The conservation laws at and the kinetics of the moving interface are incorporated into the diffusion equations and the kinetic equations of phase-field variables that are formulated for the whole system but not each domains. There are no boundary conditions at the interface and the evolution of the system is described in the absence of non-linear equations of interface kinetics. Because of its particular advantage over the sharp interface models,

<sup>1</sup> This interface kinetic model is derived from the linear but not the non-linear thermodynamics and does not consider the effect of solute diffusion in solid [3].

## Nomenclature

### Variables

$c$	overall solute concentration
$c_i, c_i^*$	solute concentration ( $i = S, L$ )
$D$	diffusion coefficient
$D_i$	diffusion coefficient
$g_i$	molar Gibbs free energy
$\Delta g_C, \Delta g_C^*$	dissipation by interface migration
$\Delta g_D, \Delta g_D^*$	dissipation by trans-interface diffusion
$F$	free energy function
$\tilde{F}$	generalized free energy function
$\tilde{F}_{out}$	total free energy production outside the system
$\tilde{F}_{in}$	total free energy production inside the system
$f$	free energy density
$f_{intf}$	interface contribution to $f$
$f_{bulk}$	bulk contribution to $f$
$f_{add}$	additional constraint contribution to $f$
$h_i$	interpolation function ( $h_S + h_L = 1$ )
$J_B$	overall solute diffusion flux
$J_B^i, J_B^{i*}$	solute diffusion flux
$J_C$	crystallization flux
$J_D$	trans-interface diffusion flux
$J_F$	projection of free energy flux vector
$l_i$	solute diffusion length
$M_c$	mobility of overall solute diffusion
$M_{cS}$	mobility of solute diffusion in solid
$M_{cL}$	mobility of solute diffusion in liquid
$M_\phi$	mobility of phase-field propagation
$n$	normal vector of the outer surface
$P$	interface permeability
$Q$	total free energy dissipation
$R$	gas constant
$T$	temperature
$t$	time
$V$	interface velocity
$V_0$	up limit of $V$
$V_{DI}$	interfacial solute diffusion velocity
$V_m$	partial molar volume
$X_k$	driving forces ( $k = \phi, J_B^S, J_B^L$ )
$\Omega$	volume of the system
$\Sigma$	outer surface of the system
$\mu_j^i, \mu_j^{i*}$	chemical potential ( $j = A, B$ )
$\mu_j^{ie}$	equilibrium chemical potential
$\tilde{\mu}$	overall solute diffusion potential
$\tilde{\mu}_i, \tilde{\mu}_i^*$	solute diffusion potential
$\Delta\mu_j, \Delta\mu_j^*$	chemical potential difference ( $\mu_j^S - \mu_j^L, \mu_j^{S*} - \mu_j^{L*}$ )

$\phi_S(\phi)$	phase-field variable of solid
$\phi_L$	phase-field variable of liquid
$\eta$	interface thickness
$\sigma_{SL}$	interface energy
$\sigma_F$	local free energy production
$\lambda$	associated Lagrange multiplier
$\psi_i$	grand potential ( $g_i - \tilde{\mu}_i c_i$ )
$\Psi$	grand potential function

### Superscripts and subscripts

$S$	solid
$L$	liquid
$A$	solvent
$B$	solute
*	value at the interface

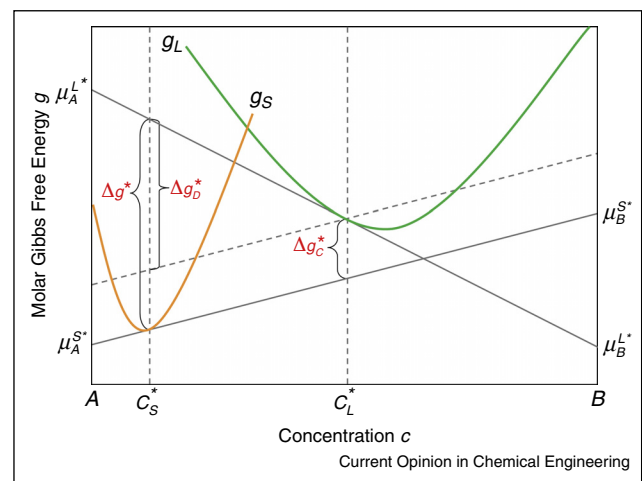
phase-field modeling is now widely used in solidification, solid-state phase transformation and so on [1,2,5–8]. It is not only a powerful simulation tool to predict the microstructure evolution but also a useful theoretical method to study the interface kinetics.

### Problem statement and motivation

This paper focuses on the phase-field modeling of isothermal solidification of binary alloys. The free energy function  $F$  is defined as

$$F = \int_{\Omega} f d\Omega = \int_{\Omega} (f_{intf} + f_{bulk}) d\Omega \quad (5)$$

Figure 1



Molar Gibbs energy diagram for the isothermal solidification of a binary alloy system [2,3]. The total Gibbs energy dissipated by the interface for solidification of one mole liquid is  $\Delta g^* = c_S^* \Delta\mu_B + (1 - c_S^*) \Delta\mu_A$ . By translating the tangent of  $g_S$  at concentration  $c_S^*$  to the point of  $g_L$  at concentration  $c_L^*$ ,  $\Delta g^*$  is divided into the dissipations by interface migration  $\Delta g_C^* = c_L^* \Delta\mu_B^* + (1 - c_L^*) \Delta\mu_A^*$  and trans-interface diffusion ( $\Delta g_D^* = (c_L^* - c_S^*) (\Delta\mu_A^* - \Delta\mu_B^*)$ ).

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