Methods for simulating the α-γ migration in ternary and multicomponent systems

Introductory presentation for discussion

n ALEMI Workshop
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What do we want?

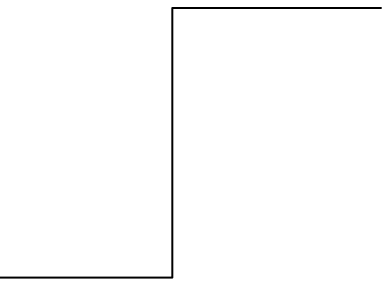
- Migration rate as function of alloy composition, temperature and time.
- Morpholgy?
- Effect of various physical effects:
  - Diffusion
  - Solute drag
  - Finite interface mobility
  - Stresses
  - External fields (magnetic fields)
  - ...

Methods to simulate migrating interfaces

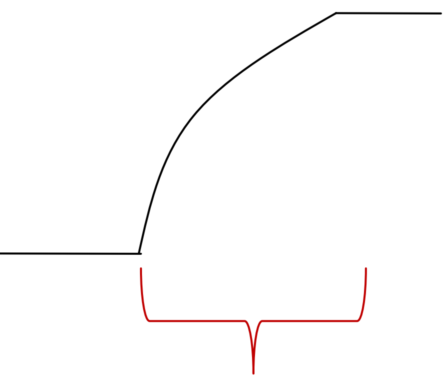
Special class of mathematical problems introduced by Josef Stefan, Slovene physiscist, 1890, who modeled ice formation - the Stefan problem

- Sharp interface
  - Front tracking
  - No front tracking
- Diffuse interface
  - Phase field
  - Level set

Sharp-interface methods



- No thickness
  - Interface is just a discontinuous change in state (variables), e.g. density, atomic arrangement, composition.
  - Some properties may be given to the interface, e.g. interfacial energy, representative composition, dissipation due to interfacial reactions, e.g. interface mobility.



- Finite thickness
  - Interface has a finite but well defined thickness
  - Properties (but not necessarily their derivatives) vary continously between the two phases.

Sharp interface – front tracking

- The position of interface is obtained as a function of time usually from velocity.
- Equation(s) for the interface velocity needed. For example from,
  - Flux balances (conservation laws)

    $$v\Delta c_k = \Delta J_k$$

  - Extremum principle

    $$v = f(\text{driving force})$$

- Usually special conditions are assumed at interface (LE, NPLE, PARA etc)

Sharp interface – no front tracking

- No special equation for the interface velocity.
- No special treatment of the interface.
- Position of interface is calculated afterwards (in each time step) by a simple equation.

Sharp interfaces +/-

+ Relatively easy to use in 1D
+ Sometimes exact or approximate analytical solutions
+ Possible to add effect interfacial energy, finite interface mobility (mixed mode), solute drag.
- Difficult to apply in general 2- or 3D cases.
- Difficulties with convergency when special conditions used at interface.

Examples of sharp interface methods

DICTRA (front tracking):

- Local equilibrium and diffusion control.
- Calphad description and mobilities needed.
- Full numerical solution of multicomponent 1D diffusion in planar, cylindrical or spherical symmetry.
- Possible to account for finite interface mobility, interface energy and elastic energy (in a simplified way).
- Possible to apply PARA conditions.

Examples of sharp interface methods

MATCALC (front tracking):

- Based on extremum principle.
- Calphad description and mobilities needed.
- No calculation of local equilibrium
- No detailed solution of diffusion profiles – steady state solutions.
- Possible to account for finite interface mobility, interface energy and elastic energy (in a simplified way).

Examples of sharp interface methods

Larsson-Hillert, 2005 (no front tracking):

- Based on absolute reaction rate theory.
- Calphad description and mobilities needed.
- No special treatment of interface
- Numerical solution of diffusion profiles by finite volume method.
- Possible to account for finite interface mobility, interface energy and elastic energy (in a simplified way).

Examples of sharp interface methods

Chen et al. 2008 (front tracking):

- Calphad description and mobilities needed.
- No detailed solution of diffusion profiles – modified steady state solutions.
- Equations for interface – flux balances are expressed in terms of mobilities and chemical potential differences.
- Possible to account for finite interface mobility, interface energy and elastic energy (in a simplified way).

Examples of sharp interface methods

Odqvist et al. 2002 (front tracking – finite thickness):

- Calphad description and mobilities needed.
- Detailed solution of diffusion profiles inside interface
- Account for finite interface mobility, interface and disipation by difusion inside interface.
- Coupled to DICTRA but problems with convergency.

Solute drag and interface mobility in simplest sharp interface model

Combination with finite interface mobility yields:

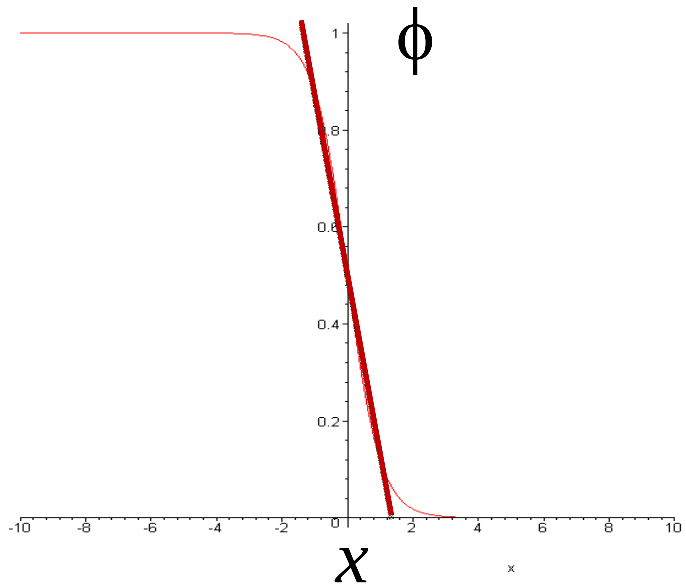
$$\Delta\mu_A = \frac{v}{V_m}\left[\frac{V_m{}^2}{M} + \frac{x_B^{\gamma/\alpha}}{L_{BB}}\left(x_B^{\gamma/\alpha} - x_B^{\alpha}\right)\right]$$

$$\Delta\mu_B = \frac{v}{V_m}\left[\frac{V_m{}^2}{M} - \frac{(1 - x_B^{\gamma/\alpha})}{L_{BB}}\left(x_B^{\gamma/\alpha} - x_B^{\alpha}\right)\right]$$

$\Delta\mu_A$ and $\Delta\mu_B$ are functions of the composition on each side of the interface and may be described by suitable thermodynamic models of the γ and α phase, respectively. If $\Delta\mu_A$ and $\Delta\mu_B$ vanish -> Local eq.

Diffuse interface methods (van der Waals) – phase field

- Continuum method – not atomistic-
- Properties vary gradually from one phase to the other.
- In a strict sense no well defined thickness of the phase interface.



$$\delta \cong (d\phi / dx)^{-1}$$

A set of partial differential equations

- Cahn-Hilliard type of equations for conserved quantities, e.g. molar fractions.
- Cahn-Allen-Ginzburg-Landau equations for non-conserved quantities, e.g. type of phase (for example $\phi = 1$ for ferrite and $\phi = 0$ for austenite)
- Equations obtained from a Gibbs energy functional.

The Gibbs energy functional:

$$G = \int_{\Omega} \left(G_m(\phi_j, x_k)/V_m + f(\text{quadratic of } \nabla\phi_j, \nabla x_k) \right) d\Omega$$

Other energy contributions, e.g. elastic energy may be added.

Cahn-Hilliard equation:

$$\dot{c}_k = \nabla \cdot \left[\sum L_{kj} \nabla \left(\frac{\delta G_m}{\delta x_j} \right) \right]$$

AC/GL-equation:

$$\dot{\phi}_j = -M_{\phi_j} \frac{\delta G}{\delta \phi_j}$$

Two methods to express: $G_m(\phi_j, x_k)$

1. Warren-Boettinger:

$$G_m(\phi\ , x_k) = f(\phi)G_m^{\alpha}(x_k) + (1 - f(\phi))G_m^{\beta}(x_k) + g(\phi)w(x_k)$$

f and g polynomials in ϕ.

2. Kim - Steinbach:

$$G_m(\phi\ , x_k) = f(\phi)G_m^{\alpha}(x_k^{\alpha}) + (1 - f(\phi))G_m^{\beta}(x_k^{\beta}) + g(\phi)w$$

$$\partial G_m^{\alpha} / \partial x_k^{\alpha} = \partial G_m^{\beta} / \partial x_k^{\beta}$$

$$x_k = f(\phi)x_k^{\alpha} + (1 - f(\phi))x_k^{\beta}$$

Several methods to express: f(quadratic of $\nabla\phi_j, \nabla x_k$)

Level set

- Not so much used in materials science but popular among mathematicians.
- Introduce a function $\phi(x,t)$. The position of interface is then defined by $\phi(x,t) = const$.
- Difficult to enter the appropriate physics.