The Phase Field Method

To simulate microstructural evolutions in materials

Nele Moelans

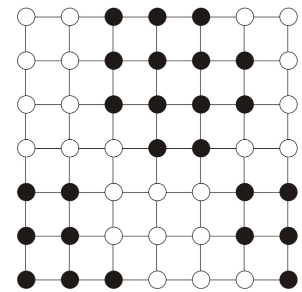
Group meeting 8 June 2004

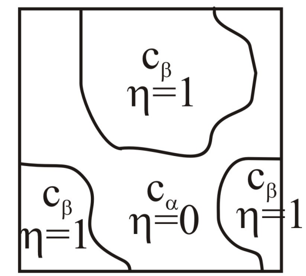
Outline

- Introduction
- Phase Field equations
- Phase Field simulations
- Grain growth
- Diffusion couples
- Conclusions

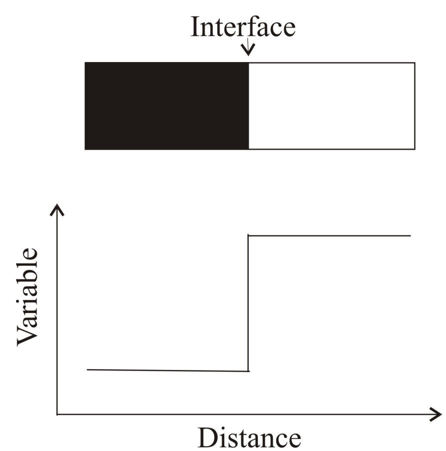
Introduction Phase Field Methode

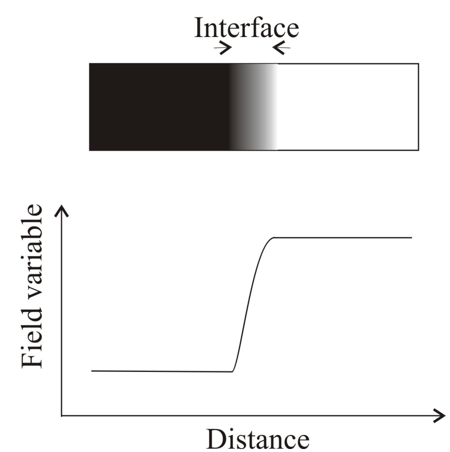
- Phase Field variables
  - Composition: c, x
  - Structure: ϕ, η





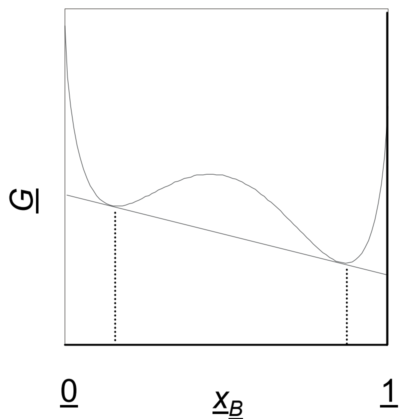
- Continuous variation in time and space
  - => no boundary conditions at moving interfaces
  - => diffuse interfaces

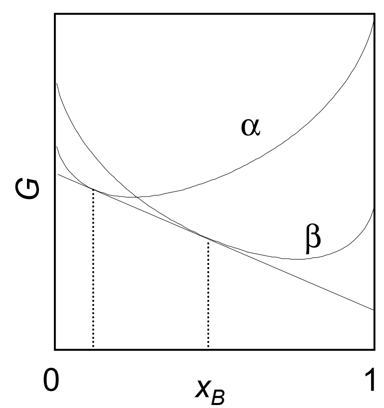




Thermodynamics for phase equilibria

- *T,p,c* constant
- CALPHAD-method
  - Thermodynamic function : $G_m(T, p, x_k)$
  - Minimization of G_m at *T,p* $\Rightarrow$ thermodynamic equilibrium
  - G_m-expressions according to thermodynamic models
  - Optimization of parameters using experimental data



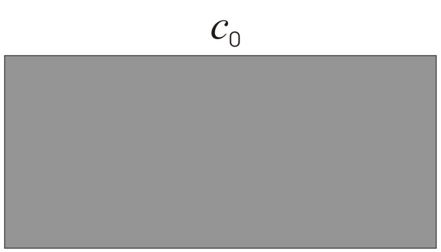


$$G(x_A, x_B, T) = x_A G_A + x_B G_B + RT(x_A \ln(x_A) + x_B \ln(x_B)) + x_A x_B L(x_A, x_B, T)$$

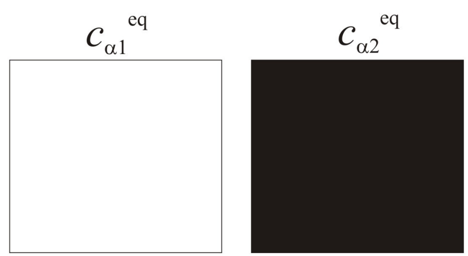
Thermodynamics of heterogeneous systems

- Homogeneous versus heterogeneous systems:

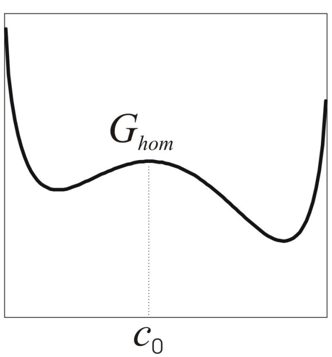
Homogeneous system

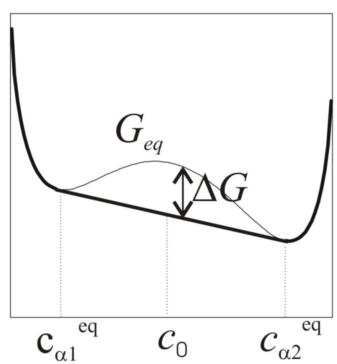


Sharp interface
Homogeneous phase



Heterogeneous system
with diffuse interface





$$G_{het}=G_{hom}+G_{grad}=G_{eq}+G_{bound}$$

Gibbs energy for heterogeneous systems

- Cahn-Hilliard (1958) $G = \int_V \left[g_{hom}(c) + \kappa(\nabla c)^2 \right] dV$

$$G = \int_V \left[g_{hom}(c,\eta) + \kappa(\nabla c)^2 + \alpha(\nabla \eta)^2 \right] dV$$

- Several contributions to Gibbs' energy

$$g_{hom}(c,\eta) = g_{chem}(c,\eta) + g_{elast}(c,\eta) + g_{mag}(c,\eta) + \ldots$$

- Interface energy flat surface

$$\sigma = \int_{-\infty}^{+\infty} \left[\Delta g(c) + \kappa\left(dc/dx\right)^2 \right] dx$$

Equilibrium for heterogeneous systems

- Conserved variables: $\frac{\partial G}{\partial c} = cte$

$$\Rightarrow \quad \frac{\partial G}{\partial c} = \frac{\partial f_{hom}}{\partial c} - 2\kappa\nabla^2 c = \mu_{hom} - 2\kappa\nabla^2 c = cte$$

- Non-conserved variables: $\frac{\partial G}{\partial \phi} = 0$

$$\Rightarrow \quad \frac{\partial G}{\partial \phi} = \frac{\partial g_{hom}}{\partial \phi} - 2\alpha\nabla^2 \phi = 0$$

Linear kinetic theory

- c,x conserved
  - Mass balance: $$\frac{\partial c_k}{\partial t} = -\nabla \cdot \vec{J}_k$$
  - Onsager: $$\vec{J}_k = -\sum_j M_{jk} \nabla \mu_j$$
- η, ϕ not conserved

$$\frac{\partial \eta}{\partial t} = -L \frac{\partial G}{\partial \eta}$$

Phase Field equations

- Cahn-Hilliard

$$\frac{\partial c}{\partial t} = \nabla \bullet M \nabla \left[\frac{\partial g_{hom}}{\partial c} - 2\kappa \nabla^2 c \right] \left(+ \zeta(\vec{r}, t) \right)$$

- Time dependent Ginzburg-Landau

$$\frac{\partial \eta}{\partial t} = -L \left(\frac{\partial g_{hom}}{\partial \eta} - 2\alpha \nabla^2 \eta \right) \left(+ \zeta(\vec{r}, t) \right)$$

- Cahn-Allen

$$\frac{\partial \phi}{\partial t} = -L \left(\frac{\partial g_{hom}}{\partial \phi} - 2\alpha \nabla^2 \phi \right)$$

Phase Field simulations

- Phase field equations

$$\frac{\partial c}{\partial t} = \nabla \cdot M \nabla \left[\frac{\partial g_{hom}}{\partial c} - 2\kappa \nabla^2 c \right]$$

$$\frac{\partial \eta}{\partial t} = -L \left(\frac{\partial g_{hom}}{\partial \eta} - 2\alpha \nabla^2 \eta \right)$$

- Determination of parameters
- Numerical solution of partial differential equations

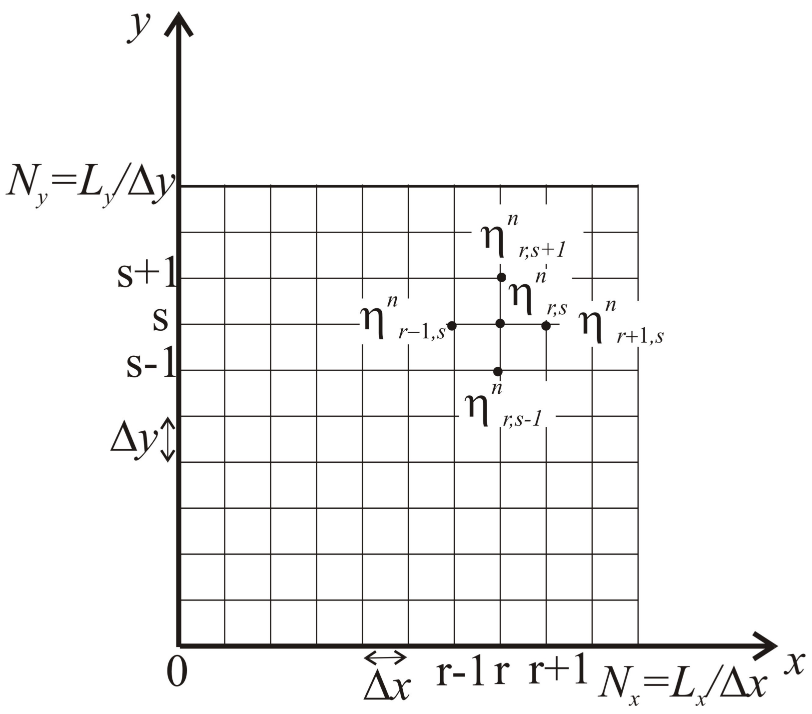
Phase Field simulations for real materials

- A lot of phenomenological parameters
  - Phase equilibria
  - Influence of inhomogenieties
  - Kinetic properties

$$\frac{\partial c}{\partial t} = \nabla \cdot M(c,\eta)\nabla\left[\frac{\partial g_{hom}(c,\eta)}{\partial c} - 2\kappa(c,\eta)\nabla^2 c\right]$$

$$\frac{\partial \eta}{\partial t} = -L(c,\eta)\left(\frac{\partial g_{hom}(c,\eta)}{\partial \eta} - 2\alpha(c,\eta)\nabla^2 \eta\right)$$

Numerical solution



- Discretisation in time and space
  - Algebraic set of (non-linear) equations
  - For each phase field variable: Nx*Ny unknowns
- Discretisation techniques
  - finite differences
  - finite elements
  - spectral methods

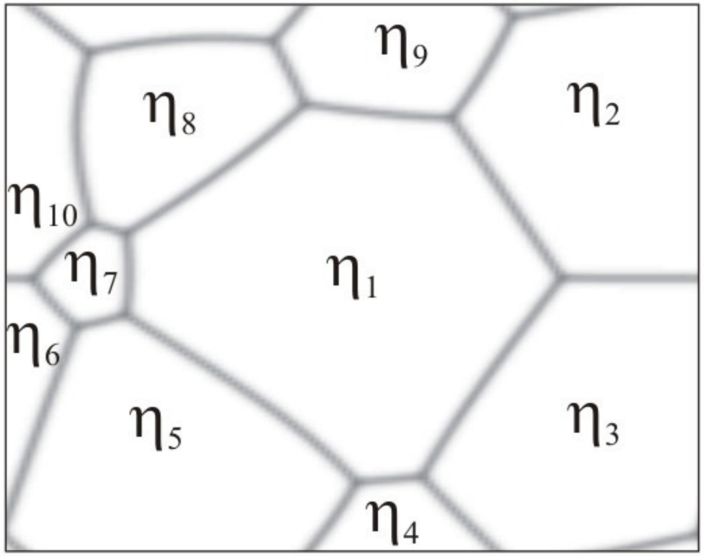
Grain Growth

- Model of D. Fan
  - Phase field variables: η_i
  - Gibbs energy

$$g_{\text{hom}} = \sum_{i=1}^{p}\left(\frac{\eta_i^4}{4} - \frac{\eta_i^2}{2}\right) + 2 * \sum_{i=1}^{p}\sum_{\substack{j=1 \\ j\neq i}}^{p} \eta_i^2 \eta_j^2$$

  - Minima

$(\eta_1,\eta_2,\ldots,\eta_p)=(1,0,0,\ldots,0),(0,1,0,\ldots,0),\ldots,(0,0,\ldots,1),(-1,0,\ldots,0),\ldots$



Grain Growth

- Influence second phase particles
  - Variable: ϕ
    - Particle: ϕ=1
    - Outside particle: ϕ=1
  - Minima Gibbs energy

    $(\phi, \ \eta_1,\eta_2,\ldots,\eta_p)=(\mathbf{1}, 0,0,\ldots 0),$

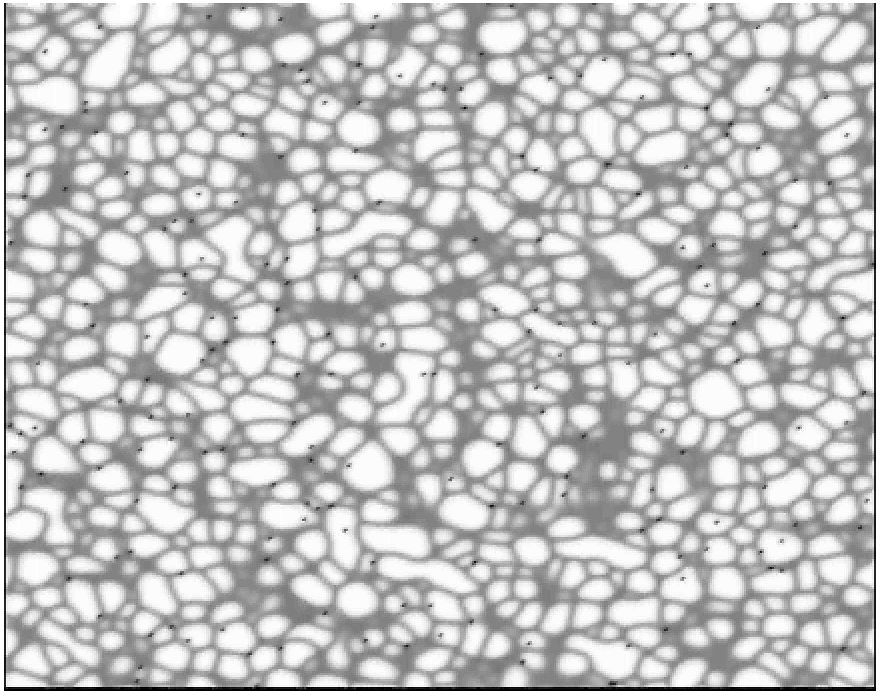
    $(\mathbf{0}, 1,0,\ldots,0),(\mathbf{0}, \ 0,1,\ldots,0),\ldots$

Grain Growth

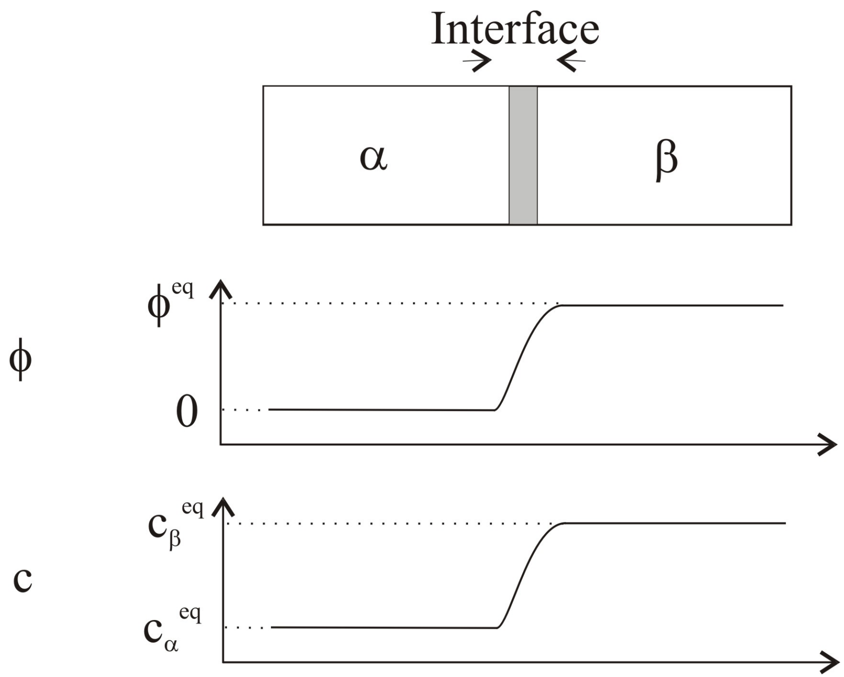
- Evolution second phase particles
  - Composition variable: c
    - Particle: $c=c_{particle}$
    - Outside particle: $c=c_{matrix}$
  - Minima free energy

    $(c, \eta_1,\eta_2,\ldots,\eta_p)=(c_{particle}, 0,0,\ldots 0),$
    $(c_{matrix}, 1,0,\ldots,0),(c_{matrix}, 0,1,\ldots,0),\ldots$
  - Precipitation, coarsening, dissolution of particles
  - Solute drag

Grain Growth simulation



Diffusion couples



- Adjustable complexity
- Coupling with CALPHAD and DICTRA

  ⇒strategy to determine parameters
- Technically relevant
- Theoretical insights

Phase equilibria: coupling with CALPHAD

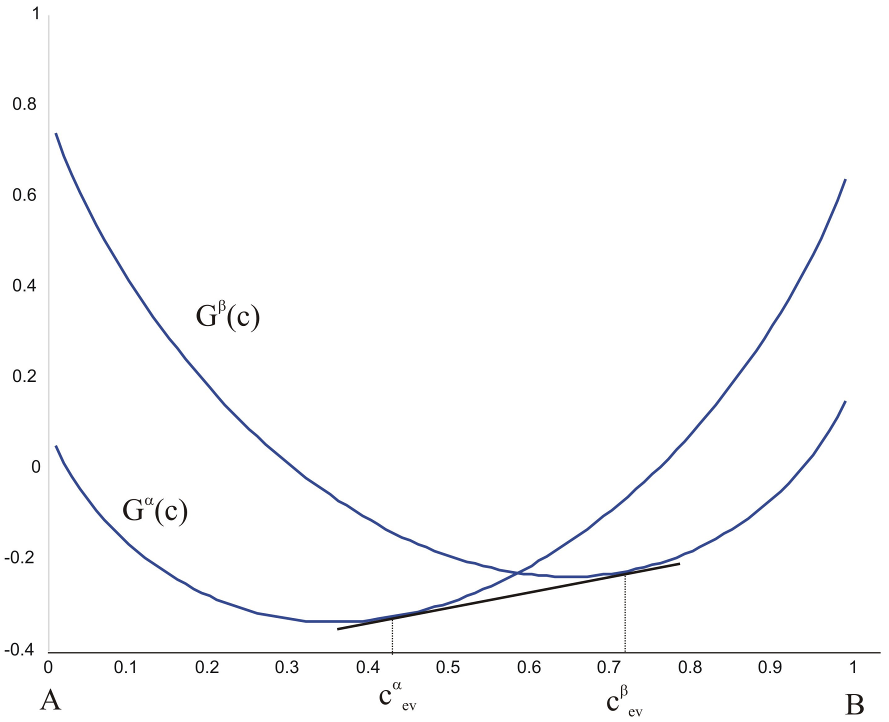
- CALPHAD

$$g(c,0,T) = \frac{G_m^{\alpha}(c,T)}{V_m}$$

$$g(c,1,T) = \frac{G_m^{\beta}(c,T)}{V_m}$$

- Phase field

$$g(c,\phi,T)$$

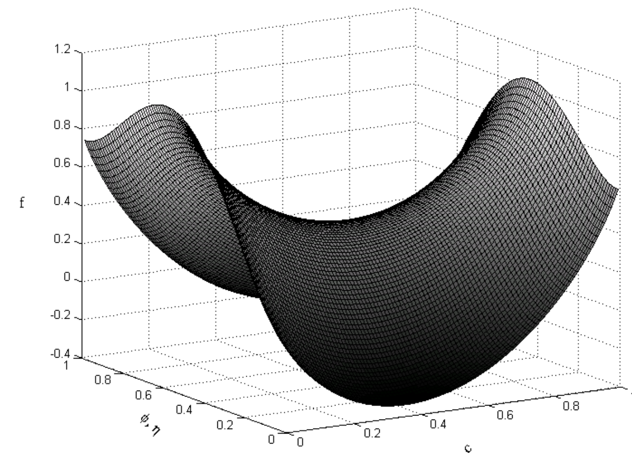


Coupling with CALPHAD

- Phenomenological phase field variables

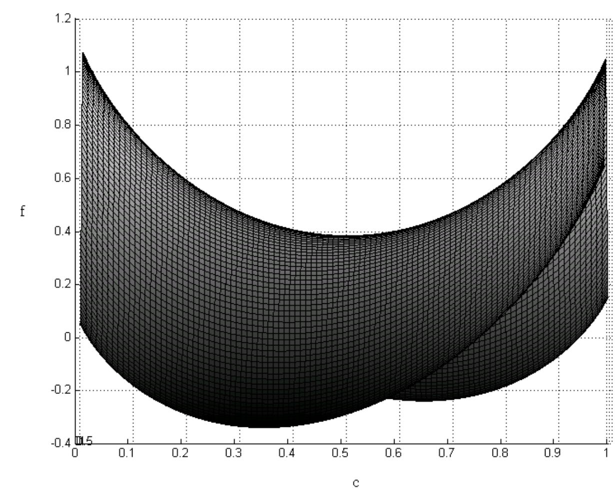
$$G_m(c_k,\phi)=\left(1-p(\phi)\right)G_m^{\alpha}(c_k)+p(\phi)G_m^{\beta}(c_k)+g(\phi)W(c_k)$$

  - $p(\phi)=\phi^2(3-2\phi)$
  - $g(\phi)=\phi^2(1-\phi)^2$



- Physical order parameters
  - Landau expansion polynomial

$$g(c,\eta_k)=g(c,0)+\sum_i B_i(c)\eta_i+\sum_{ij} C_{ij}(c)\eta_i\eta_j+\sum_{ijk} D_{ijk}(c)\eta_i\eta_j\eta_k+\sum_{ijkl} E_{ijkl}(c)\eta_i\eta_j\eta_k\eta_l+\dots$$



Kinetics: coupling with DICTRA

- DICTRA
  - Diffusion in lattice reference frame: $J_k = -x_k x_{Va} \frac{\Omega_{kVa}}{V_m} \frac{\partial \mu_k}{\partial x}$
  - Atomic mobilities: $M_k = x_{Va} \Omega_{kVa}$
  - Arrhenius expression for temperature dependence:

$$M_k = \frac{1}{RT} M_k^0 \exp(-Q_k / RT)$$

$$RT \ln(RTM_k) = RT \ln(M_k^0) - Q_k = \Phi + \Theta$$

  - Redlich-Kister expansion for composition dependence:

$$\Phi_k = \sum_i x_i \Phi_{k,i}^0 + \sum_i \sum_{j>i} x_i x_j \Phi_{k,ij}$$

Kinetics: coupling with DICTRA

- Phase field
  - Onsagers' law: $$J_k = -\sum L_{ki} \frac{\partial \mu_i^{het}}{\partial x}$$
  - Laboratory reference frame
- Diffusion experiments
  - Fick's law $$J_k = -D_k \frac{\partial c}{\partial x}$$
  - Interdiffusion, tracer, intrinsic

Conclusions

- Consistent and powerful theory
- Main problems
  - Large amount of parameters to determine
  - Computer resources
- Further work
  - More efficient implementation
  - Coupling between Phase Field Method and other thermodynamic modeling techniques
  - Case studies