Phase field modelling of microstructure evolution

Nele Moelans

Department of metallurgy and materials engineering,
K.U.Leuven, Belgium

Research group: Thermodynamics in materials engineering
- Introduction on the phase field method
- Phase field simulations of grain growth
  - Zener pinning
  - Thermal grooving
- Outlook
Phase field method

- van der Waals, Cahn-Hilliard (1958), Hohenberg and Halperin (1977)

- Microstructure evolution (started ± 20 years ago)
  - Solidification
  - Ordering reactions
  - Martensitic transformation

- Nowadays
  - Wide range of applicabilities
  - Quantitative aspects
    - Parameter determination
    - Numerical implementation
Role of microstructures in materials science

Chemical composition, temperature, pressure
+
Cooling rate, history

Microstructure
Shape, size and orientation of the grains, mutual distribution of the phases

Material properties
Strength, deformability, hardness, toughness, fatigue...
Representation of microstructures in the phase-field method

- Field variables: continuous functions in space and time
  - Local composition \( x_B(r,t) \)
  - Local structure and orientation \( \eta_k(r,t) \)

Binary alloy A-B

- Phase \( \alpha \): \( \eta = 0 \)
- Phase \( \beta \): \( \eta = 1 \)

Anti-phase boundary
Diffuse-interface description

- Sharp interface
  - Discontinuous variation in properties
  - Requires tracking of the interfaces
  - Simplified grain morphologies

- Diffuse interface
  - Continuous variation in properties
  - Interfaces implicitly given by local variations in field variables
  - Complex grain morphologies
Thermodynamics and kinetics

- **Total free energy**

\[ F = F_{\text{bulk}} + F_{\text{surface}} = \int_V f_0(x_i, \eta_k, T) + \frac{K}{2} \sum_{k=1}^{p} (\nabla \eta_k)^2 + \frac{\mathcal{E}}{2} \sum_{i=1}^{C} (\nabla x_i)^2 \, dV \]

- **Evolution of field variables**

  - **Non-conserved field variables**

    \[ \frac{\partial \eta_k(\mathbf{r}, t)}{\partial t} = -L \frac{\partial F(x_1, \ldots, x_C, \eta_1, \ldots, \eta_p)}{\partial \eta_k(\mathbf{r}, t)} + \xi(\mathbf{r}, t) \]

  - **Composition fields**

    \[ \frac{1}{V_m} \frac{\partial x_i(\mathbf{r}, t)}{\partial t} = \nabla M \cdot \nabla \frac{\partial F(x_1, \ldots, x_C, \eta_1, \ldots, \eta_p)}{\partial x_i(\mathbf{r}, t)} + \xi(\mathbf{r}, t) \]
Homogeneous free energy functional

- Anti-phase boundary
Homogeneous free energy

- Two phase system
**Major strengths of the phase-field technique**

- Complex morphologies + concurrent processes

  - Continuous field representation $x_B(r, t), \eta(r, t)$

  - Several contributions to thermodynamic driving force

    $$F = F_{bulk} + F_{surface} + F_{elast} + F_{magn} + ...$$

- Kinetics
  - Mass diffusion
  - Heat diffusion (conduction)
  - Convection
Quantitative aspects

- Parameter determination
  - Thermodynamic phase stabilities
  - Interfacial energy and mobility
  - Elastic energy
  - Orientation dependence
  - Solute diffusion

- Numerical solution of a set of coupled partial differential equations

- Width of the interface
Phase field simulations of microstructural evolution

Experiments, atomistic simulations and thermodynamic models

Crystal structure, phase stabilities, interfacial properties (energy, mobility, structure, anisotropy), diffusion properties

Phase field simulations

Morphological evolution of the grains at the mesoscale during solidification, precipitation, solid-state phase transformations, grain growth, …

Models that predict macroscopic material properties

Strength, deformability, hardness, toughness, fatigue…
Phase field simulations of grain growth

- Polycrystalline microstructure (L.Q. Chen 1994):
  \[ \eta_1, \eta_2, \ldots, \eta_i(r,t), \ldots, \eta_p \]

- Grain i of matrix-phase
  \[ (\eta_1, \eta_2, \ldots, \eta_i, \ldots, \eta_p) = (0, 0, 1, \ldots, 0) \]
• **Mechanism for controlling grain size**
  - E.g. NbC, AlN, TiN,... in HSLA-steels

• **Zener relation for limiting grain size**

\[
\frac{R_{\text{lim}}}{r} = K \frac{1}{f_v^b}
\]

• **Influence of**
  - Shape of the particle
  - Interfacial properties of particles
  - Particle-grain boundary correlation
  - Initial distribution
  - Evolution particles

*Example: MnS precipitate in low-C steel*
Zener pinning

- 3D phase field simulation

Grain orientations: $\eta_1, \eta_2, \ldots, \eta_i (\vec{r}, t), \ldots, \eta_p$

Particles: $\eta_i = 0, \forall i$

Conserved variable: $\phi(\vec{r}, t)$

$\Rightarrow$ Grain size distribution

$\Rightarrow$ Limiting grain size

$\Rightarrow$ Number of particles on grain boundary
Thermal grooving

- **Surface tension**
  
- **Formation mechanism**
  - Bulk diffusion, surface diffusion, evaporation/condensation
  - Groove shape

- **Drag effect on grain growth in thin films**

- **Abnormal grain growth induced by orientation dependence of surface energy**
  
  => huge grain size

*In-situ STM image for a gold film (Rost et al. 2003)*
Thermal grooving

- 3D phase field simulation of surface grooving
  - System geometry
    - Environment
      - $\psi = 1$
      - $\eta_1 = 0$
      - $\eta_2 = 0$
    - Film
      - $\psi = 0$
      - $\eta_1 = 1$
      - $\eta_2 = 0$
    - $\eta_2 = 1$

- Model
  - Grains $\eta_1, \eta_2, \ldots, \eta_i(r, t), \ldots, \eta_p$
  - Conserved variable $\psi(r, t)$

- Application
  - Onset of abnormal grain growth
Outlook

- Quantitative simulations for multi-component and multi-phase materials
  - Model refinement
    - Easy coupling with thermodynamic databases
    - Individual parameters for interfacial energy
  - Physical characteristics

- Extension of the grain growth model
  - Stability of the particles
  - Surface properties of the particles
Outlook

- Phase field simulations for Ag-Cu-Sn
  - Multi-phase/multi-component
  - Elastic energy
  - COST 531, COST MP0602 → input parameters

- Phase field simulations for oxidic systems
  - Ions with multiple valence, e.g. Fe$^{2+}$/Fe$^{3+}$
  - Slags, ceramics
Thank you for your attention!

More information: http://nele.studentenweb.org
Arenberg Castle, Leuven, Belgium