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Modeling Factory Webinar

Phase Field modeling

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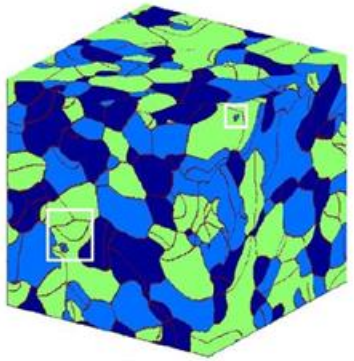
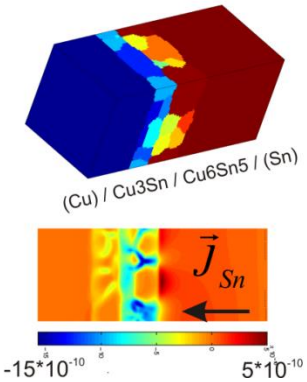
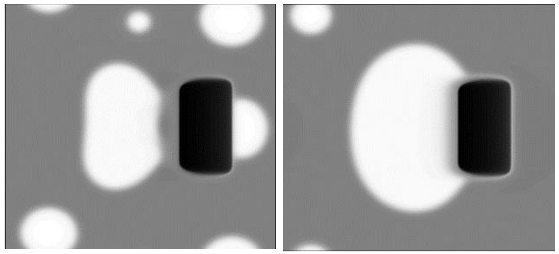
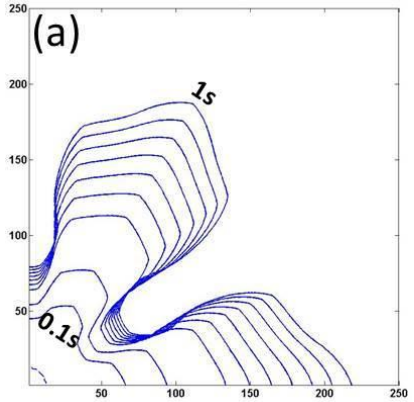
eit RawMaterials

- Dept. Materials Engineering, KU Leuven, Belgium
  - http://www.mtm.kuleuven.be/English/
- Solidification and Microstructure Simulation group
  - https://www.mtm.kuleuven.be/Onderzoek/Semper/SolMicS
- Phase-field method, multi-component alloys, microstructures









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Outline

- Phase field method
- Examples
- Ideas on data management

Phase Field Method

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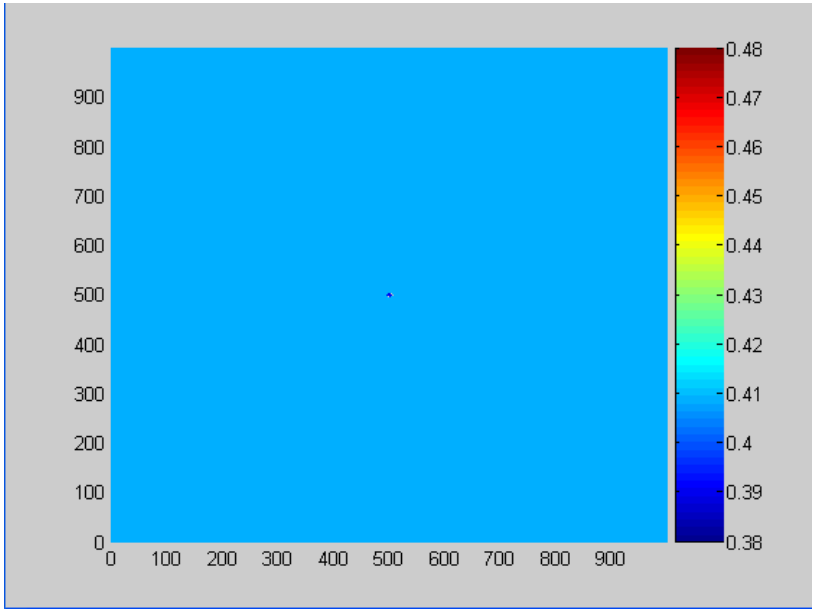
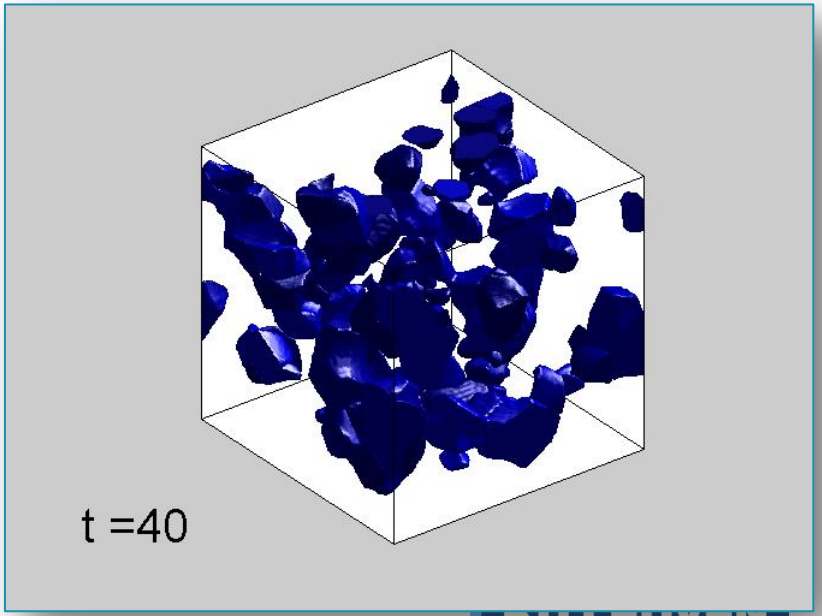
Phase-field method

- Microstructure evolution
  - Meso- & micro scale (5 nm - mm)
  - Thermodynamic principles
- Wide field of applications
  - Solidification, phase transitions, diffusion, grain growth, deformation, crack formation, ferro-electric/magnetic domains, nanoparticle, nanocrystals, thin films, ….
- Coupling with CALPHAD

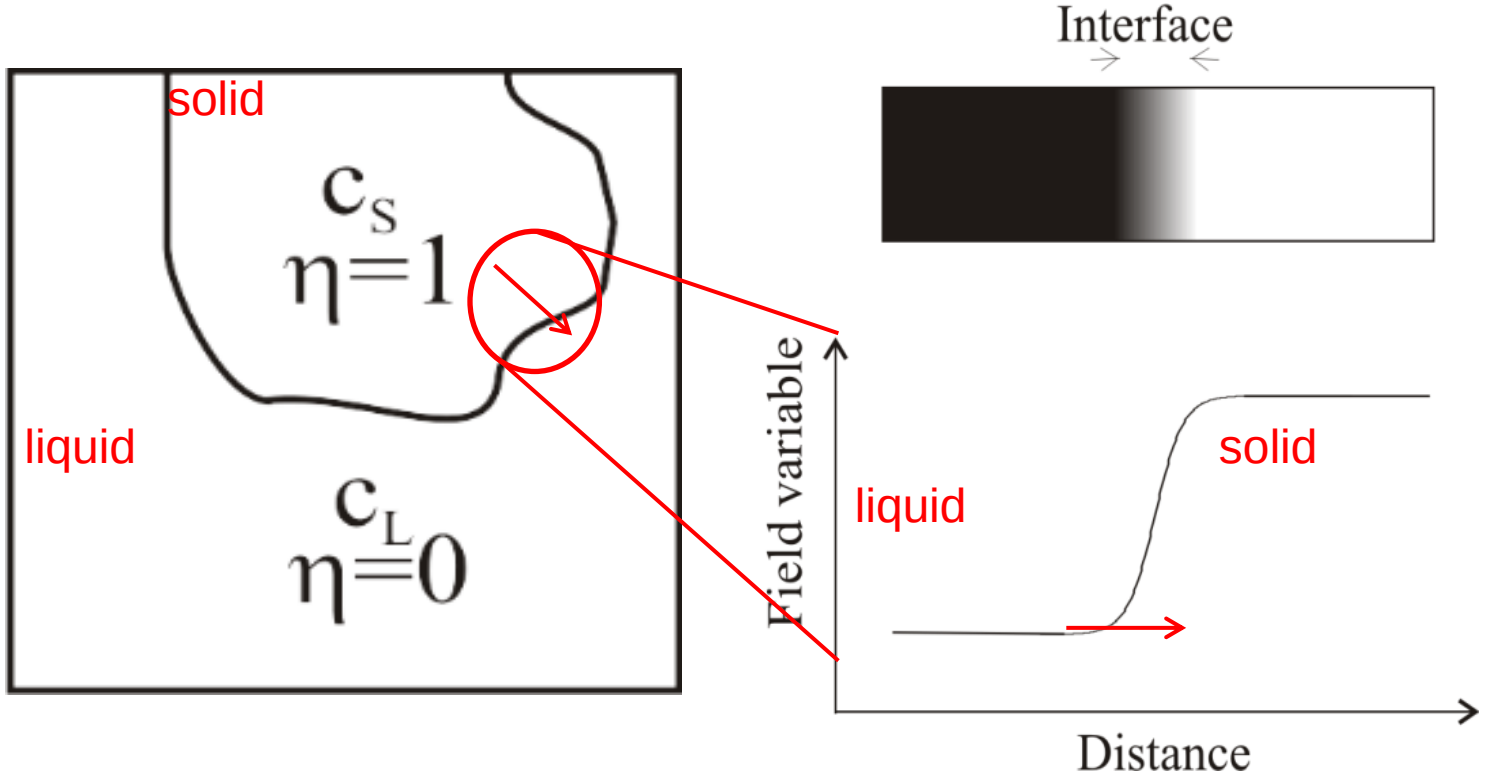
⟶ multi-component, multi-phase





Microstructure representation

- Composition: $c_k(\vec{r}, t)$
- Structure, orientation: $\eta_i(\vec{r}, t)$ or $\phi_i(\vec{r}, t)$

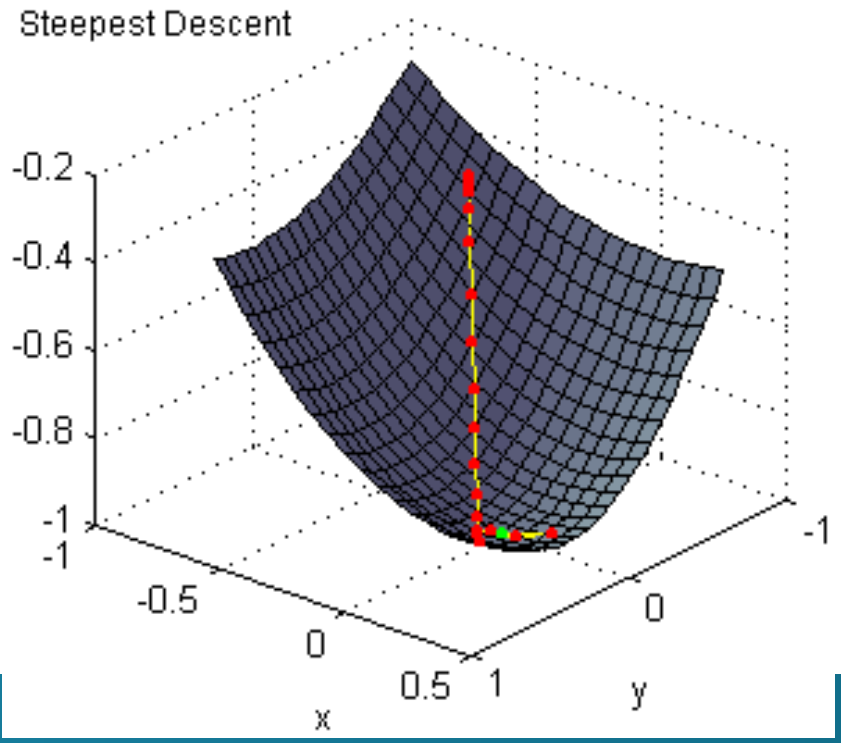


Evolution equations

- Non-conserved fields: $\eta_i(\vec{r},t)$ or $\varphi_i(\vec{r},t)$

$$\frac{\partial \varphi_i(\vec{r},t)}{\partial t} = -L\frac{\partial F(\varphi_i, c_k)}{\partial \varphi_i(\vec{r},t)} \quad (+\vartheta_i(\vec{r},t))$$

→ boundary motion



Evolution equations

- Concentration fields: $c_k(\vec{r}, t)$
  - Steepest descent + mass conservation

$$\frac{1}{V_m}\frac{\partial c_k(\vec{r}, t)}{\partial t} = \nabla M(\varphi_i, c_k)\nabla\tilde{\mu}_k \quad (+\theta_k(\vec{r}, t))$$

$$\tilde{\mu}_k = \frac{\partial F(\varphi_i, c_k)}{\partial c_k(\vec{r}, t)} = \mu_k - \mu_C$$

→ solute diffusion

Thermodynamic free energy

$$F = F_{bulk} + F_{interf}$$

$$= \int_V \left[f_0(c_k, \varphi_i) + \frac{\varepsilon_\varphi}{2} \sum_i (\nabla \varphi_i)^2 + \frac{\varepsilon_c}{2} \sum_k (\nabla c_k)^2 \right] dV$$

Homogeneous free energy

chemical, elastic, …, + double/multi-well $g(\varphi_i)$

Gradient free energy

→ diffuse interfaces

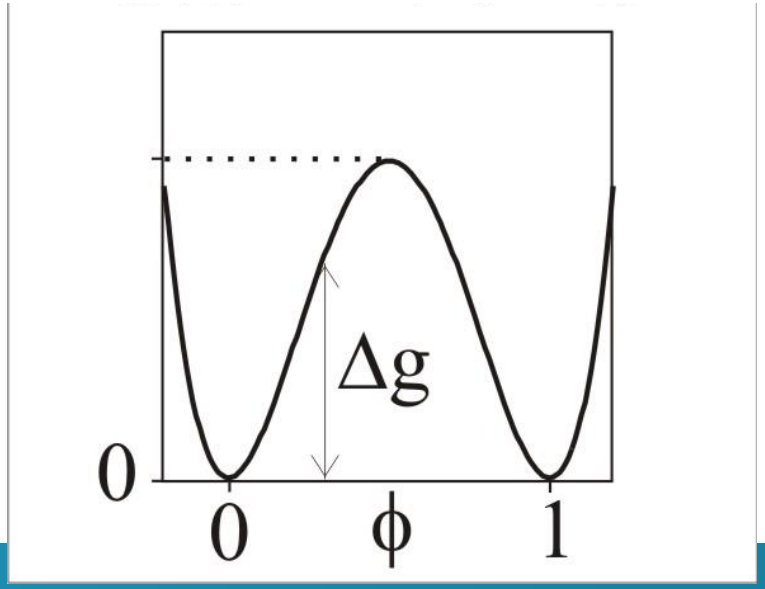
Interface energy

$$F = F_{bulk} + F_{interf}$$

$$= \int_V \left[f_0(c_k, \varphi_i) + \frac{\varepsilon_\varphi}{2} \sum_i (\nabla \varphi_i)^2 + \frac{\varepsilon_c}{2} \sum_k (\nabla c_k)^2 \right] dV$$

Double well:

$$g(\varphi) = 16W\varphi^2(1-\varphi)^2$$



Interface energy:

$$\propto \sqrt{\varepsilon_\varphi}, \sqrt{\varepsilon_c}, \sqrt{(\Delta g)_{max}}$$

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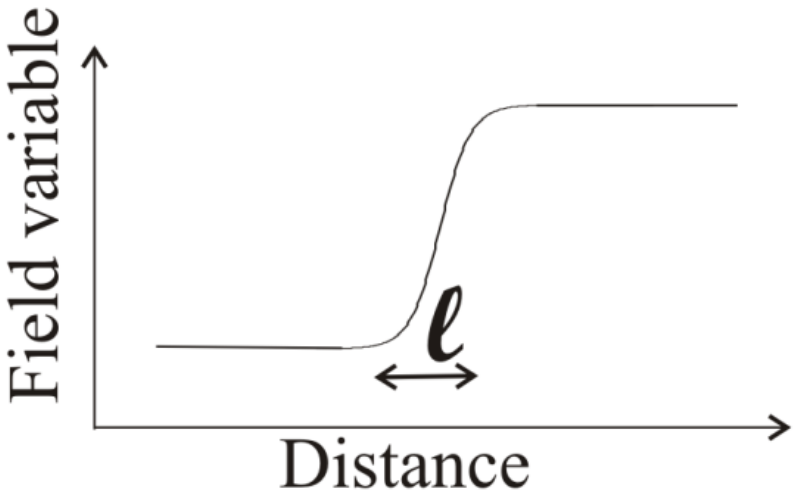
Interface width

$$F = F_{bulk} + F_{interf}$$

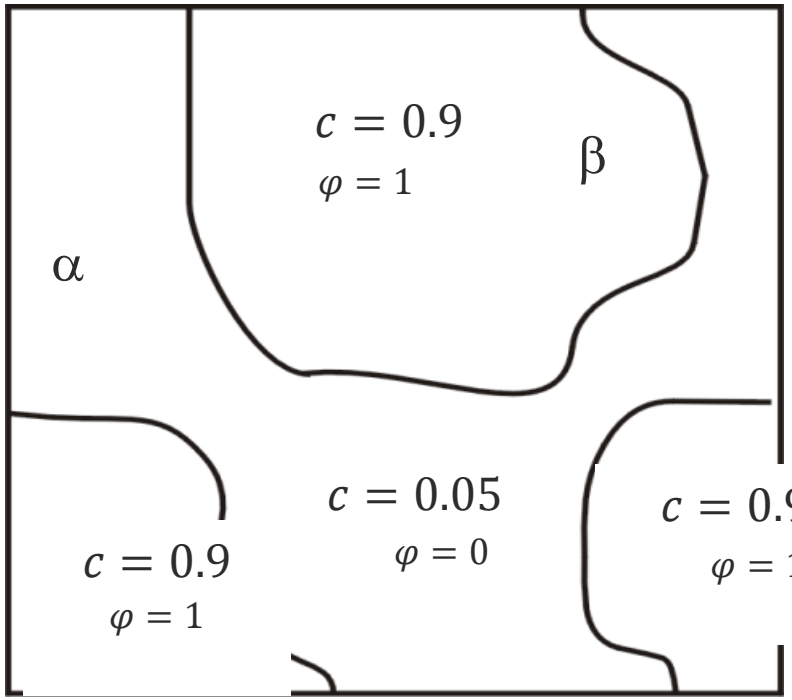
$$= \int_V \left[f_0(c_k, \varphi_i) + \frac{\varepsilon_\varphi}{2} \sum_i (\nabla \varphi_i)^2 + \frac{\varepsilon_c}{2} \sum_k (\nabla c_k)^2 \right] dV$$



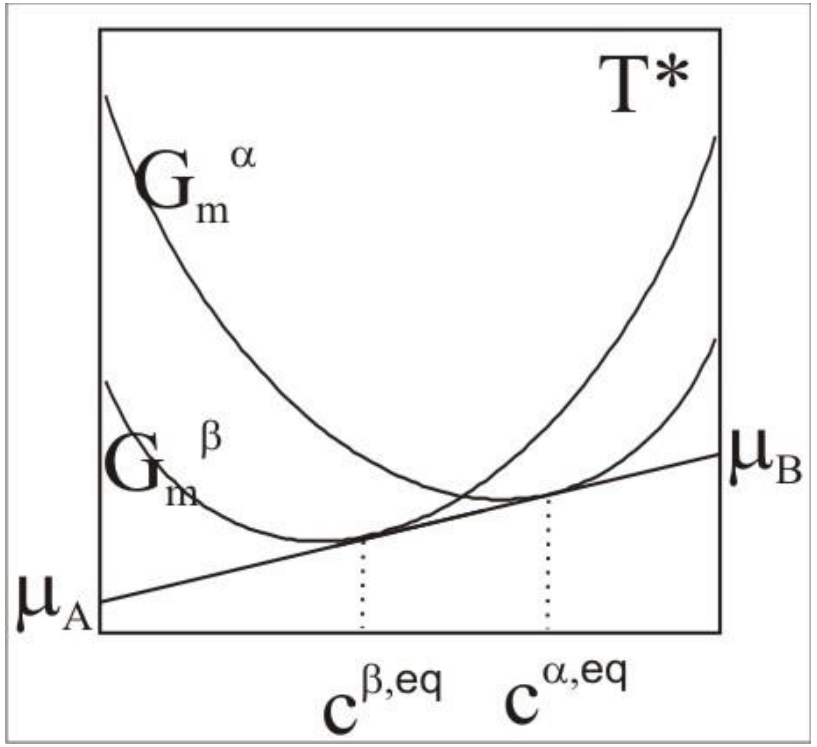
Interface width:

$$\propto \sqrt{\varepsilon_\varphi}, \sqrt{\varepsilon_c}, \sqrt{1/(\Delta g)_{max}}$$

Example: Binary 2-phase system



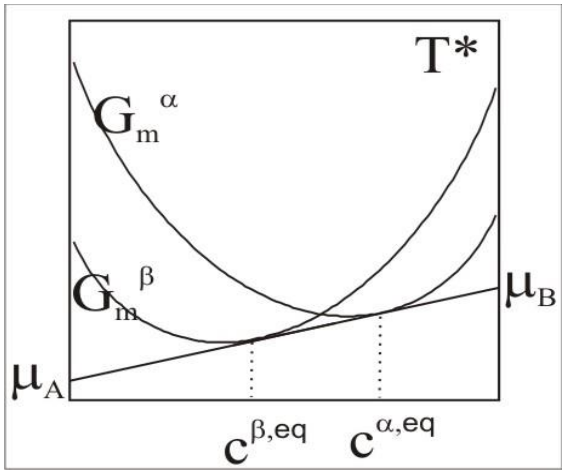
$\varphi(\vec{r}, t)$, $c(\vec{r}, t)$

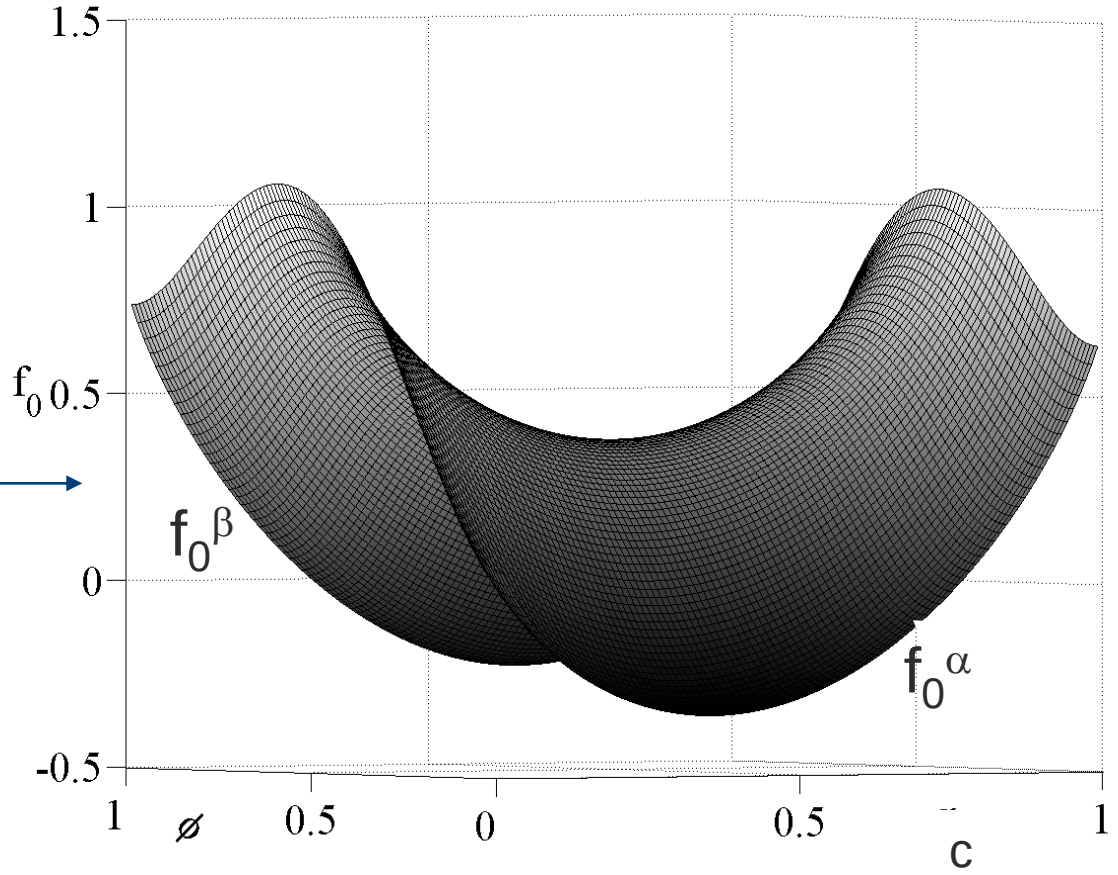


Gibbs energy α and β phase

$f_0(c, \varphi)$?

Example: Binary 2-phase system





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

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

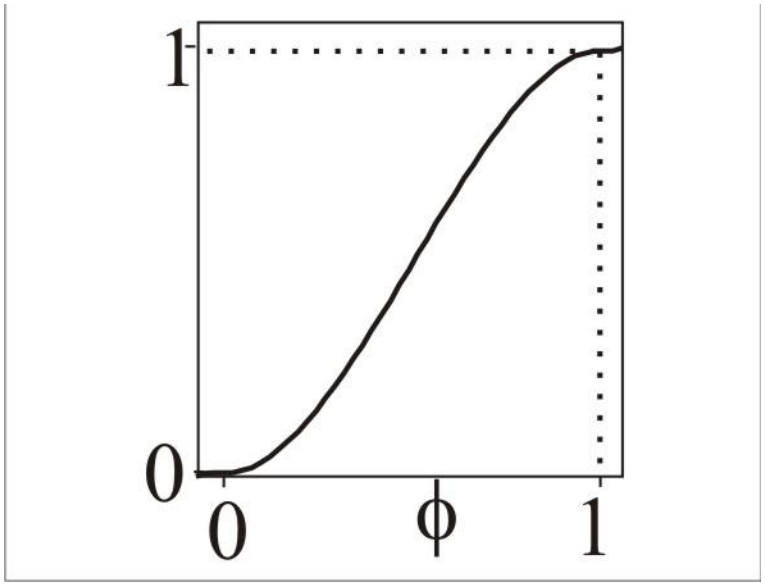
$$f_0 = h(\phi)\, f^{\beta}(c,T) + \left[1 - h(\phi)\right] f^{\alpha}(c,T) + \omega g(\phi)$$

Example: Binary 2-phase system

$$f_0 = h(\phi)\, f^{\beta}(c,T) + [1-h(\phi)]\, f^{\alpha}(c,T) + \omega g(\phi)$$

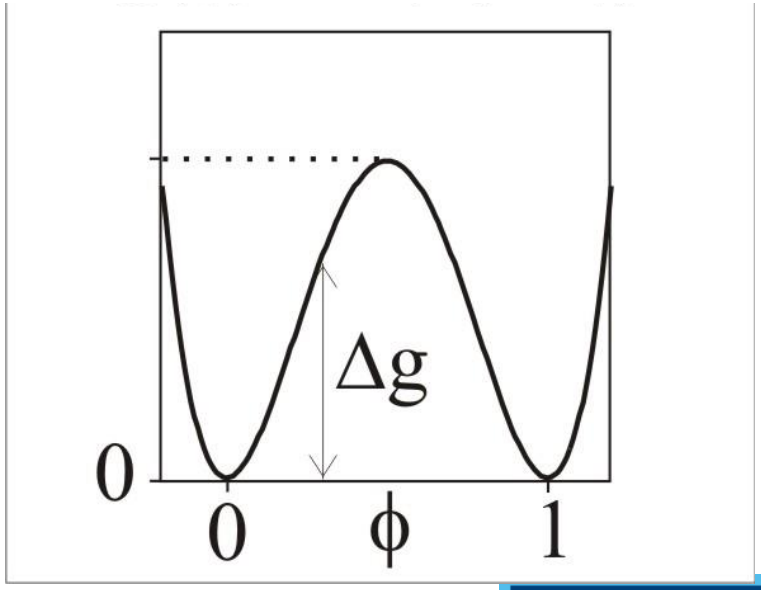
Interpolation:

$$h(\varphi) = \varphi^3(10 - 15\varphi + 6\varphi^2)$$



Double well:

$$g(\varphi) = 16W\varphi^2(1-\varphi)^2$$

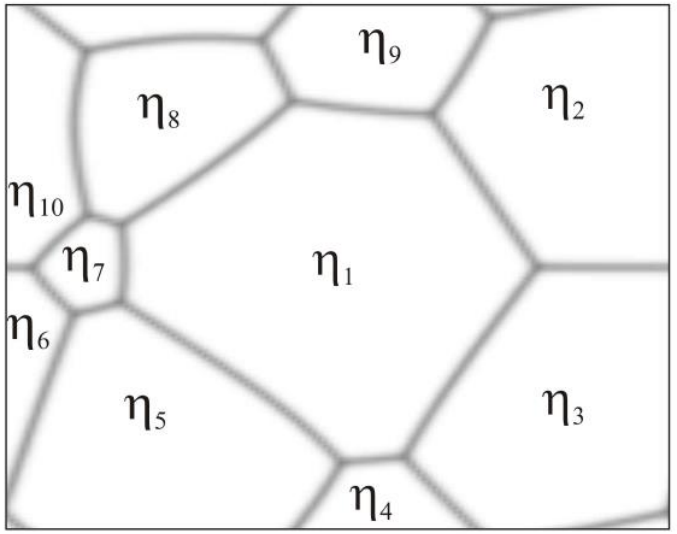


Polycrystals/multi-phase

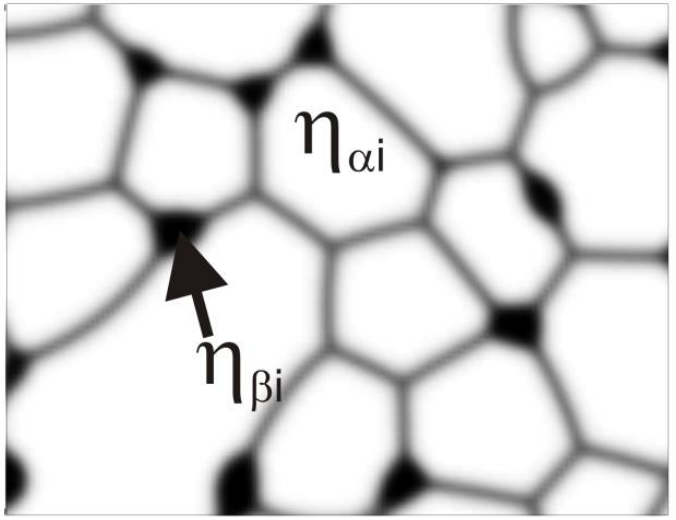
- Single phase: $\eta_1, \eta_2, \ldots, \eta_i(\vec{r}, t), \ldots, \eta_p$

within grain i

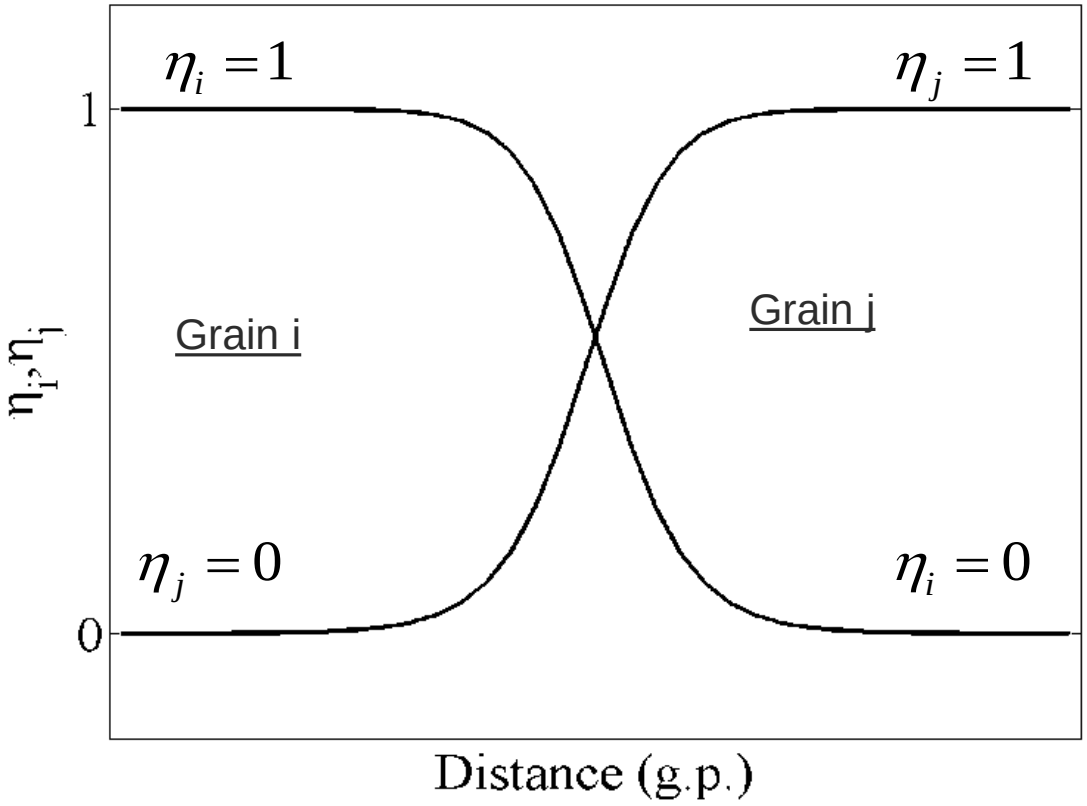
$$(\eta_1, \eta_2, \ldots, \eta_i, \ldots, \eta_p) = (0, 0, \ldots, 1, \ldots, 0)$$



- Multi-phase
  - Phases/grains $\eta_{\alpha 1}, \eta_{\alpha 2}, \ldots, \eta_{\alpha i}(\vec{r}, t), \ldots, \eta_{\beta 1}, \eta_{\beta 2}, \ldots \eta_p$
  - Composition $c_A, c_B(\vec{r}, t), \ldots, c_{C-1}$



Polycrystals/multi-phase



Other driving forces

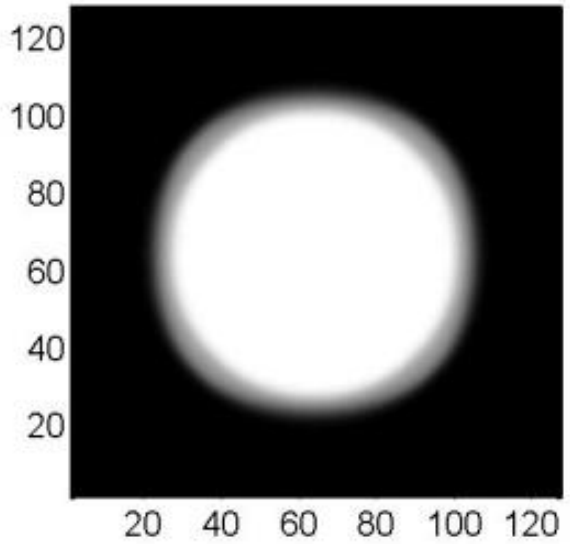
$$F = F_{chem} + F_{elast} + F_{ferromag} + \dots$$

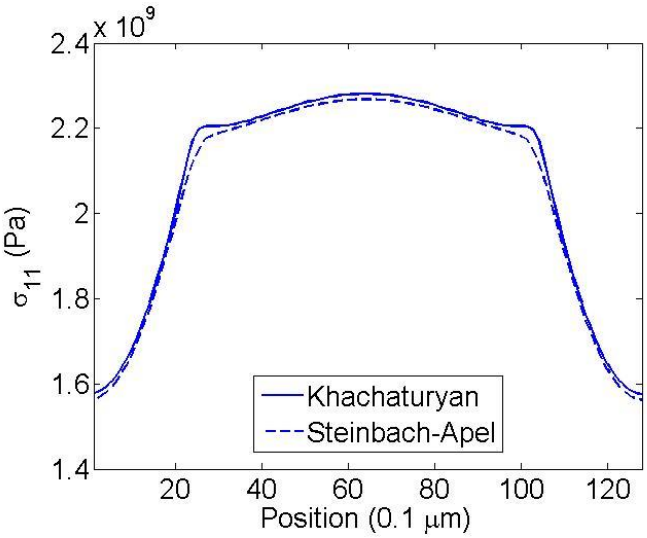
- Micro-elasticity theory

$$F_{elast} = \frac{1}{2}\int_V C_{ijkl}(\eta, x)\varepsilon_{ij}^{el}(\eta, x)\varepsilon_{kl}^{el}(\eta, x)dV$$

- Transformation, applied and thermal strains/stresses

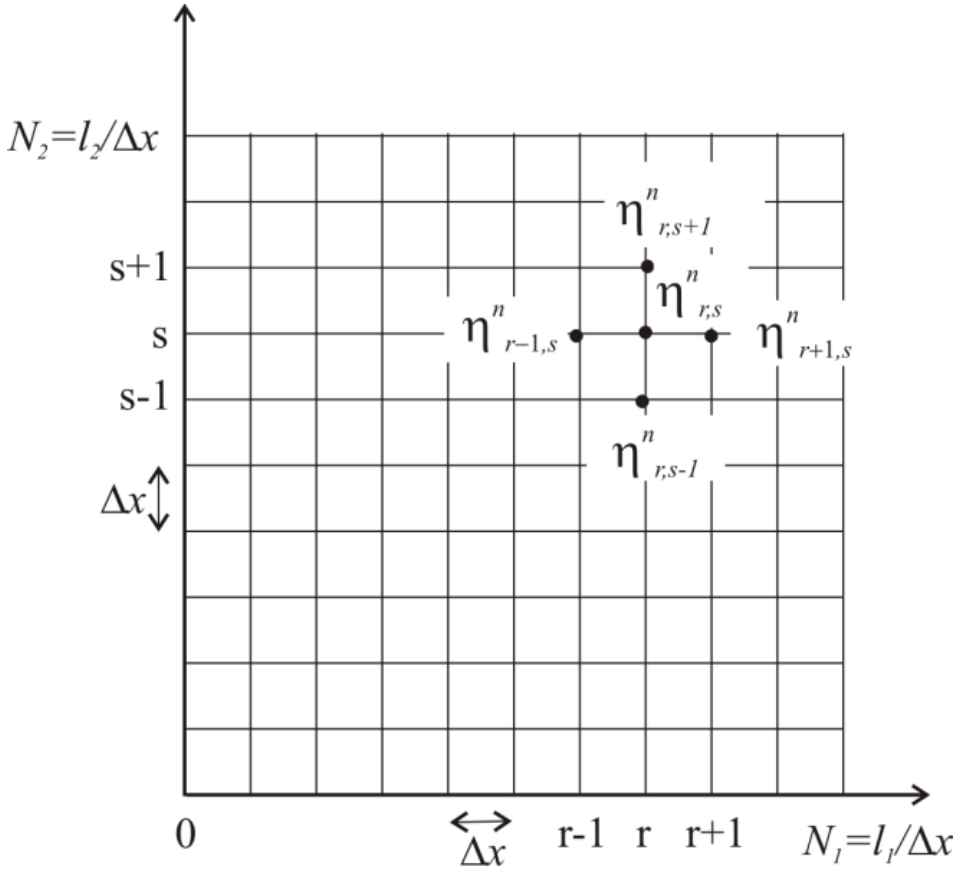
- Solid-solid transformations

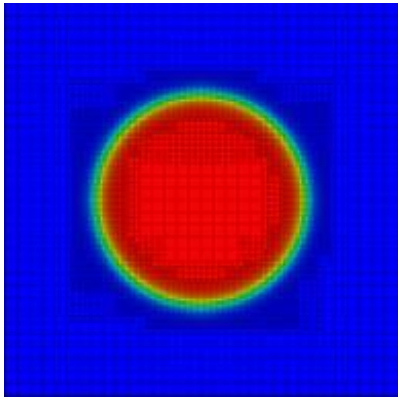


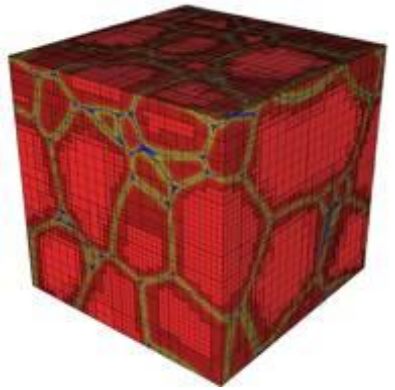


Numerical implementation

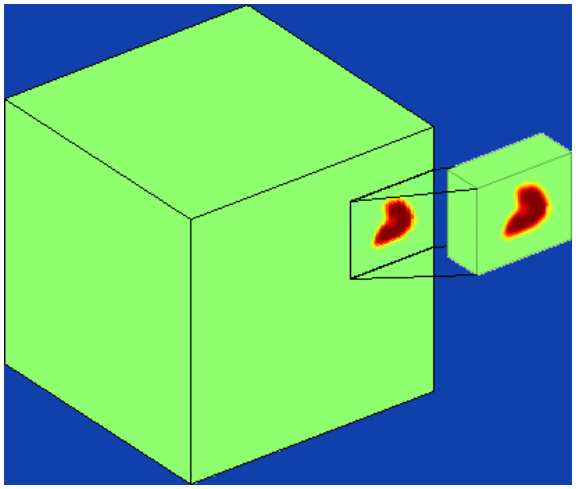
- Finite differences, finite elements, fourier-spectral







Adaptive meshing

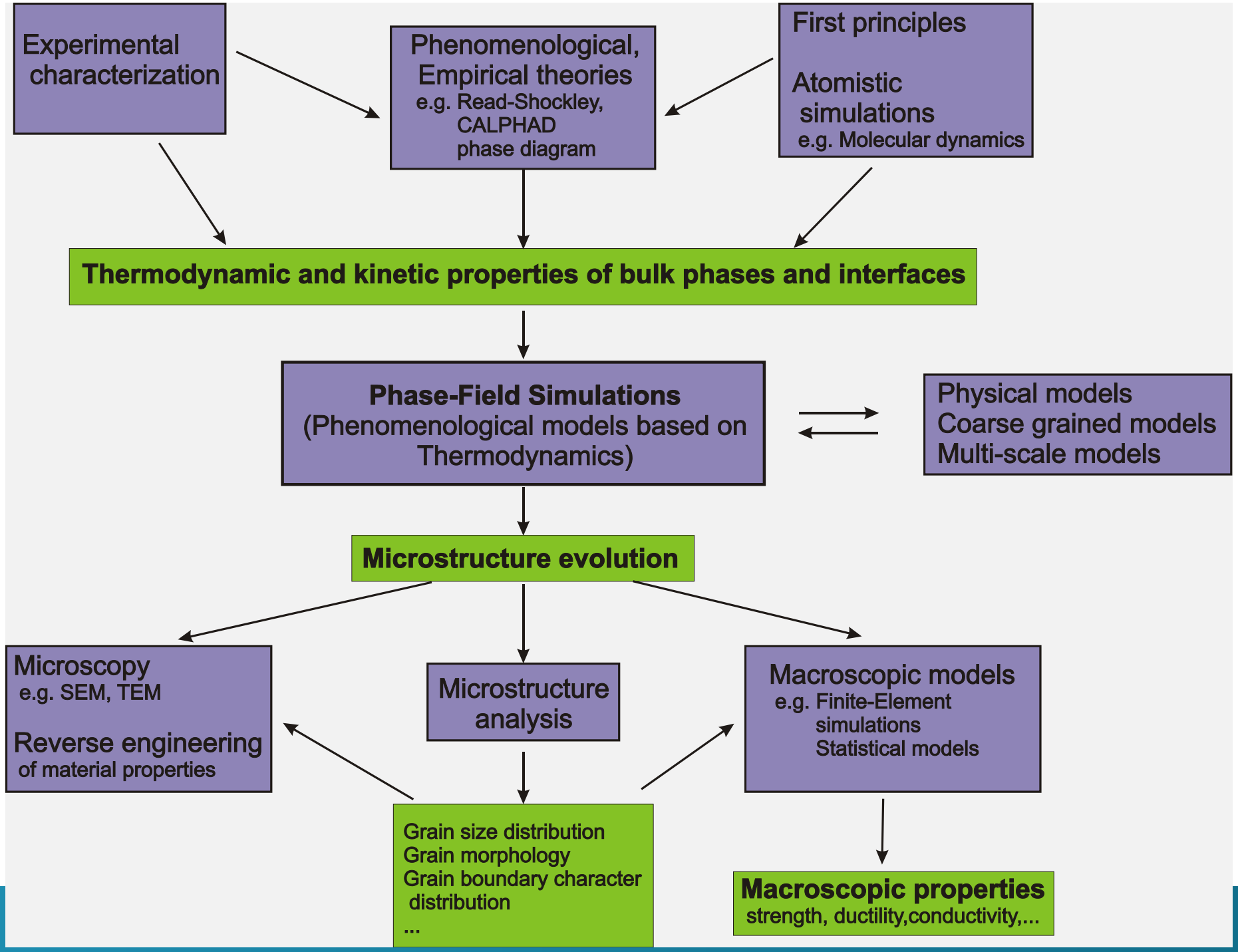


Sparse data structures

Parameter assessment

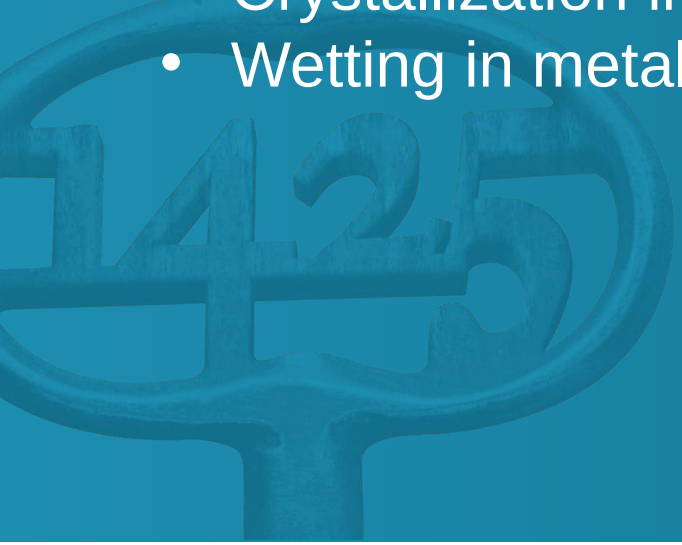
- Different kinds of input data
  - Phase stabilities, phase diagram
    - CALPHAD ← experiments, DFT
  - Interfacial energy and mobility
    - MD, DFT, experimental
  - Elastic properties, crystal structure, lattice parameters
    - ab-initio, experimental
  - Diffusion mobilities
    - DICTRA ← experimental, MC ← DFT

- Orientation and composition dependence


Experimental characterization
Phenomenological, Empirical theories
e.g. Read-Shockley, CALPHAD phase diagram
First principles
Atomistic simulations
e.g. Molecular dynamics
Thermodynamic and kinetic properties of bulk phases and interfaces
Phase-Field Simulations
(Phenomenological models based on Thermodynamics)
Physical models
Coarse grained models
Multi-scale models
Microstructure evolution
Microscopy
e.g. SEM, TEM
Reverse engineering
of material properties
Microstructure analysis
Macroscopic models
e.g. Finite-Element simulations
Statistical models
Grain size distribution
Grain morphology
Grain boundary character distribution
...
Macroscopic properties
strength, ductility,conductivity,...

Examples

- Polycrystals
- IMC growth at material interfaces
- Crystallization in oxide systems
- Wetting in metal-oxide sytems



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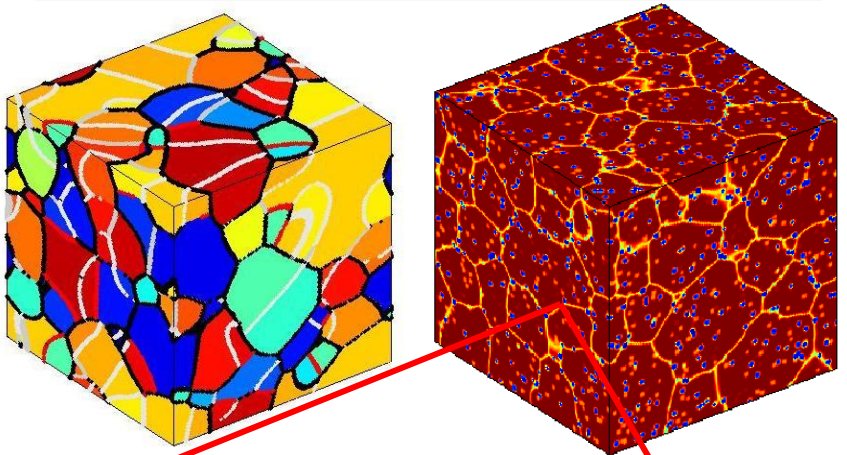
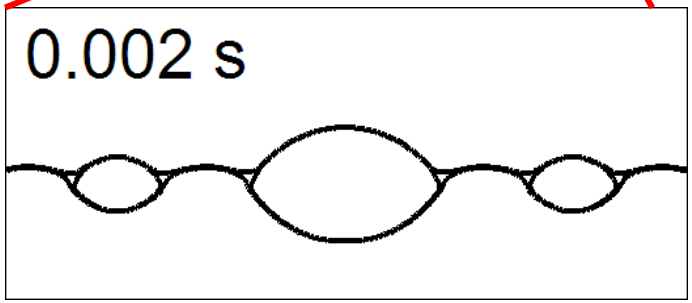
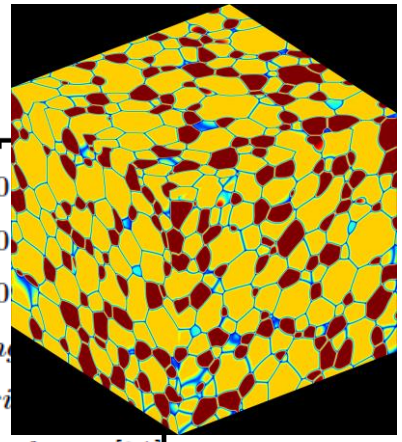
Polycrystals

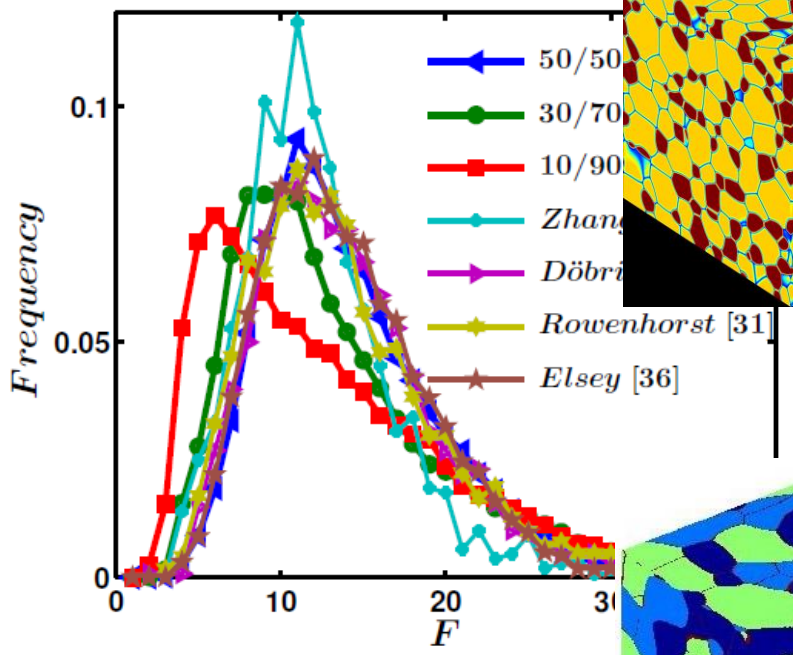
Effect of anisotropy and precipitates

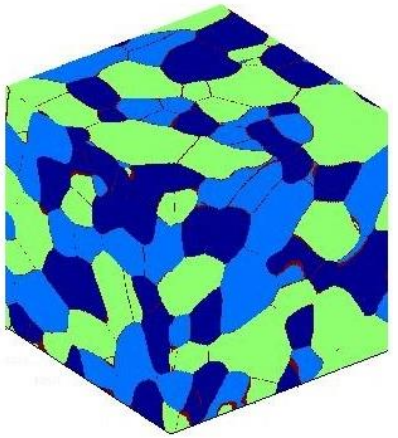


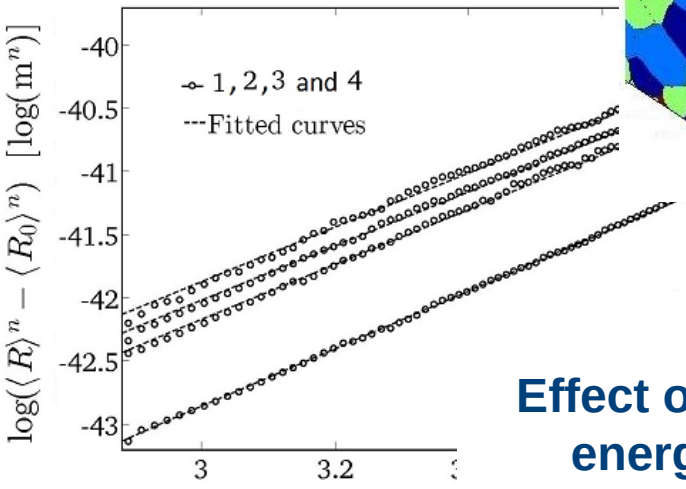


Multi-phase materials





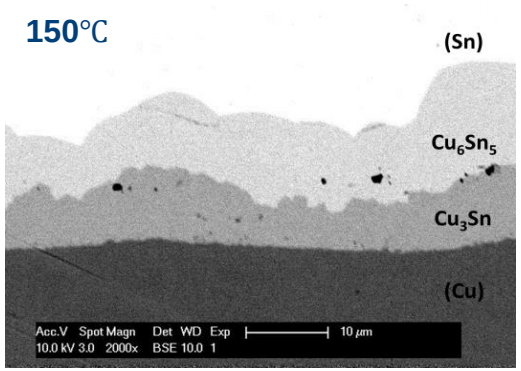




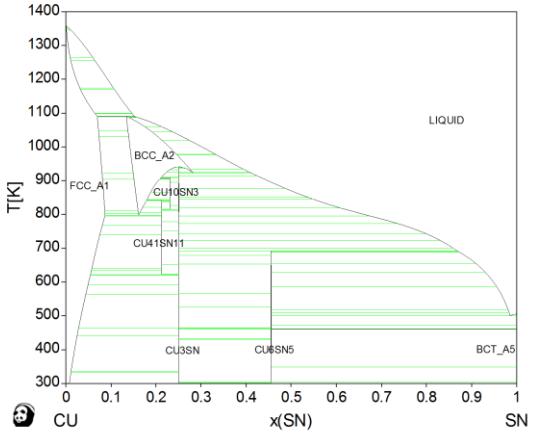
Effect of interface energies and diffusion coefficients

Modeling IMC growth

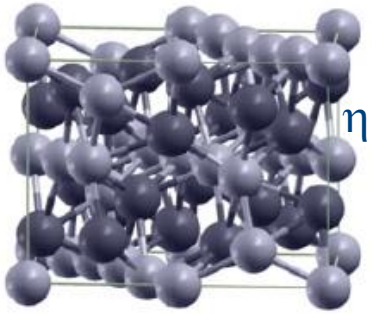
Experiments



CALPHAD/DICTRA

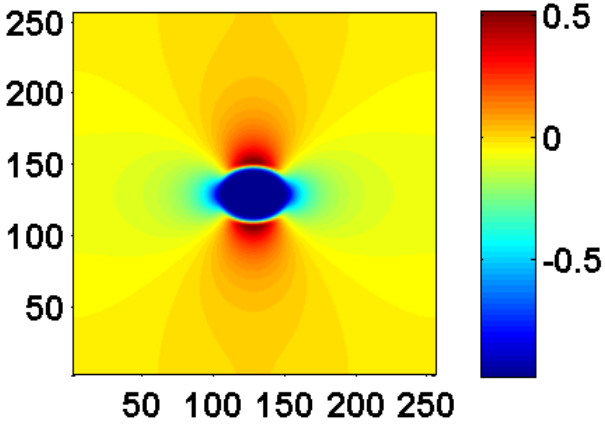


Ab initio calculations

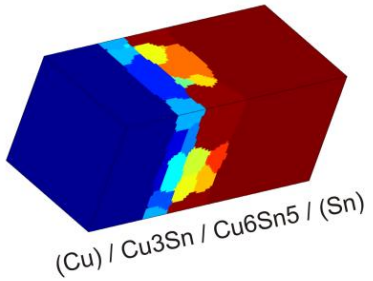


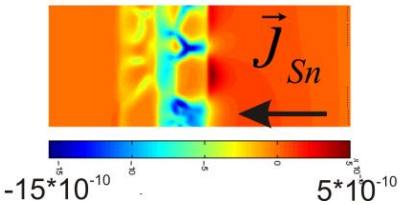
η'-cu6sn5

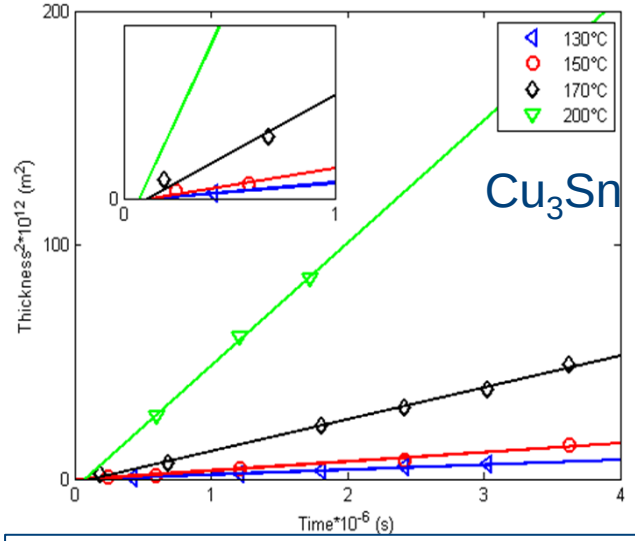
Micro-elasticity and plasticity model



Phase field simulation



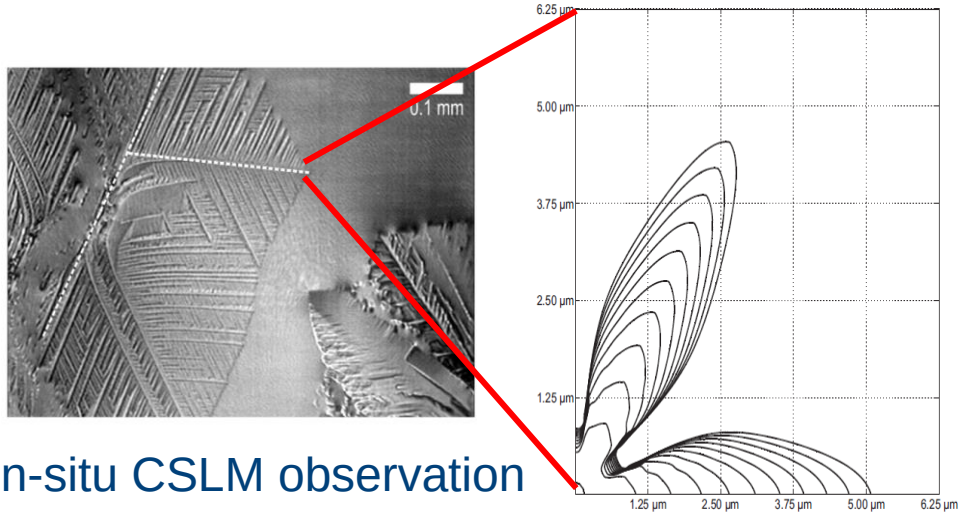




Analysis: growth rates, morphology, diffusion paths, solubilities, diffusion coefficients

Crystallization in oxide melts

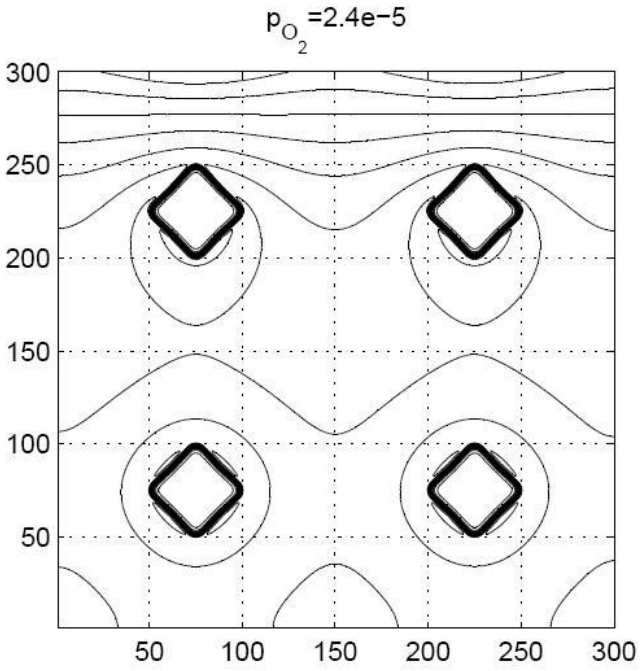
Wollastonite growth from $CaO\text{-}Al_2O_3\text{-}SiO_2$ melts



In-situ CSLM observation

Simulation

Magnetite growth in oxidizing $FeO\text{-}Fe_2O_3\text{-}SiO_2$ system



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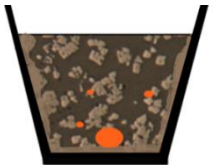
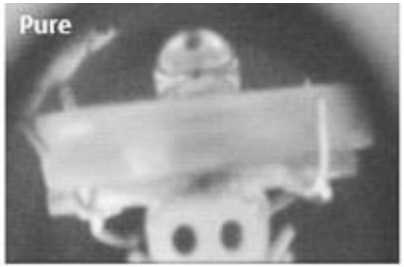
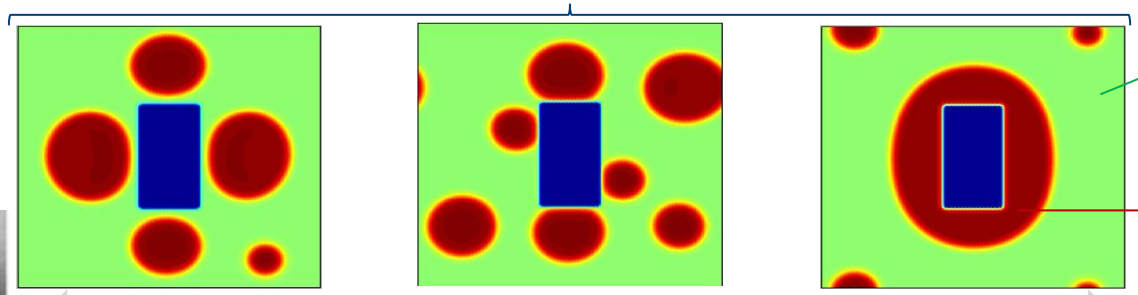
Wetting in metal-oxide systems

Sticking metal droplets







Oxide slag

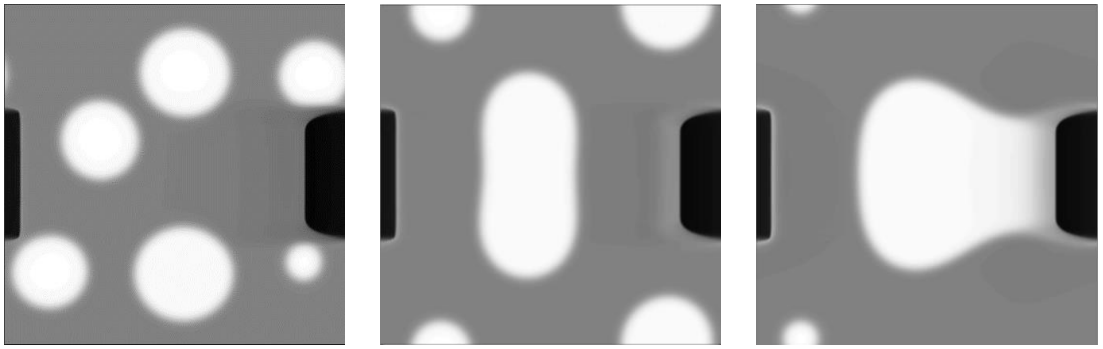
Metal droplets

Spinel particle

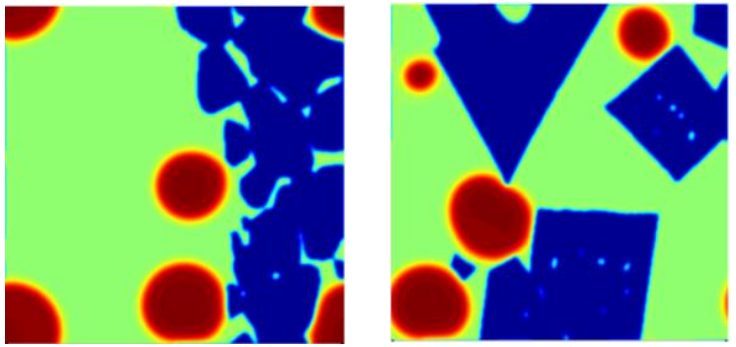
Effect of interfacial energies

$\gamma_{S,LO}$ = 1.2641N/m	$\gamma_{S,LO}$ = 1.2641N/m	$\gamma_{S,LO}$ = 1.6318N/m
$\gamma_{S,LM}$ = 4.0093N/m	$\gamma_{S,LM}$ = 2.0260N/m	$\gamma_{S,LM}$ = 1.3325N/m

Effect rigid body motion



Realistic spinel structures



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Ideas on data management

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Different kinds of data involved

- Input data
- Initial structures (files from which simulations can be started)
- Raw simulation data
- Processed simulation results
- (Simulation codes)

Input data

- Data type
  - Gibbs energy, diffusion coefficient/mobility, interface energy grain boundary energy
- Specifications
  - Temperature, composition, orientation, …
- Value
- Source
  - Reference, method
- Accuracy

Initial microstructure

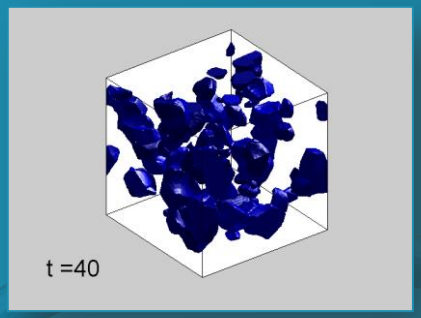
- Description
  - Number of components, grains, phases, system size, …
- Source
  - Method / how is the structure obtained, eg experimental micrograph, voronoi tesselation, ….
- Data
  - Files with the values of the phase-field variables as a function of position
    - Important to specify the format well

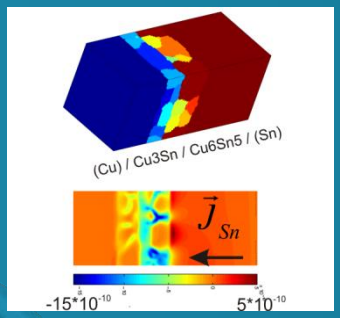
Raw simulation data

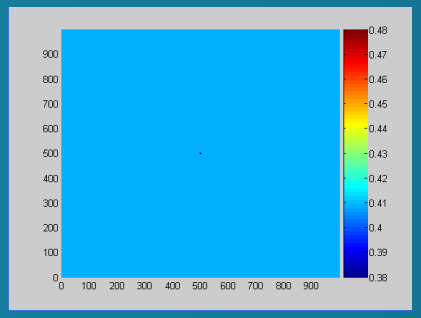
- File with (model) input data
  - Values + references
  - Or reference to ‘input data’ files
- Reference to initial structure files
- Numerical details
  - Discretization technique, name+version simulation program, time stepping, grid spacing
- Data
  - Files with the values of the phase-field variables as a function of position and time
    - Important to specify the format well

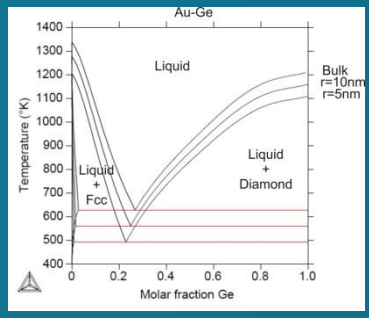
Processed simulation results

- Type
  - Images, movies, graphs, …
- Content
  - Eg mol fraction B as a function of time, grain size distribution, …
- Reference to the raw data files, input files, initial data files









https://www.mtm.kuleuven.be/Onderzoek/Semper/SolMicS

Solidification & Microstructure Simulation