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Phase-field modelling

Lecture 7 in 4H5919

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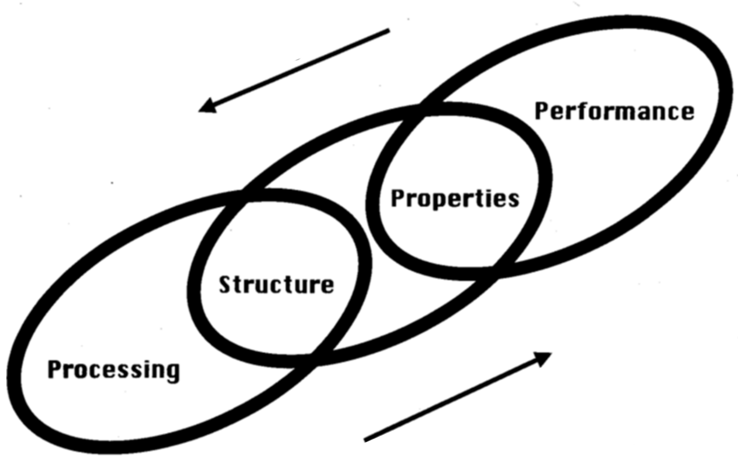
(Home assignment)

Outline

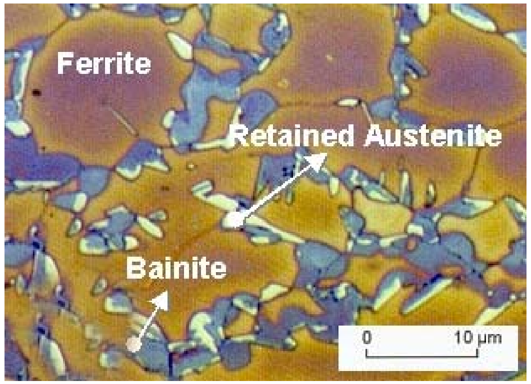
- History and background to the Phase-Field Method (PFM)
- Mathematics of the PFM
- Modelling with the PFM
- Examples of applications
- The home assignment

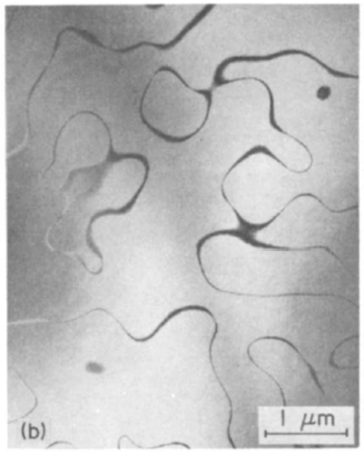
PFM in the ICME framework

- Creator – linking process with structure

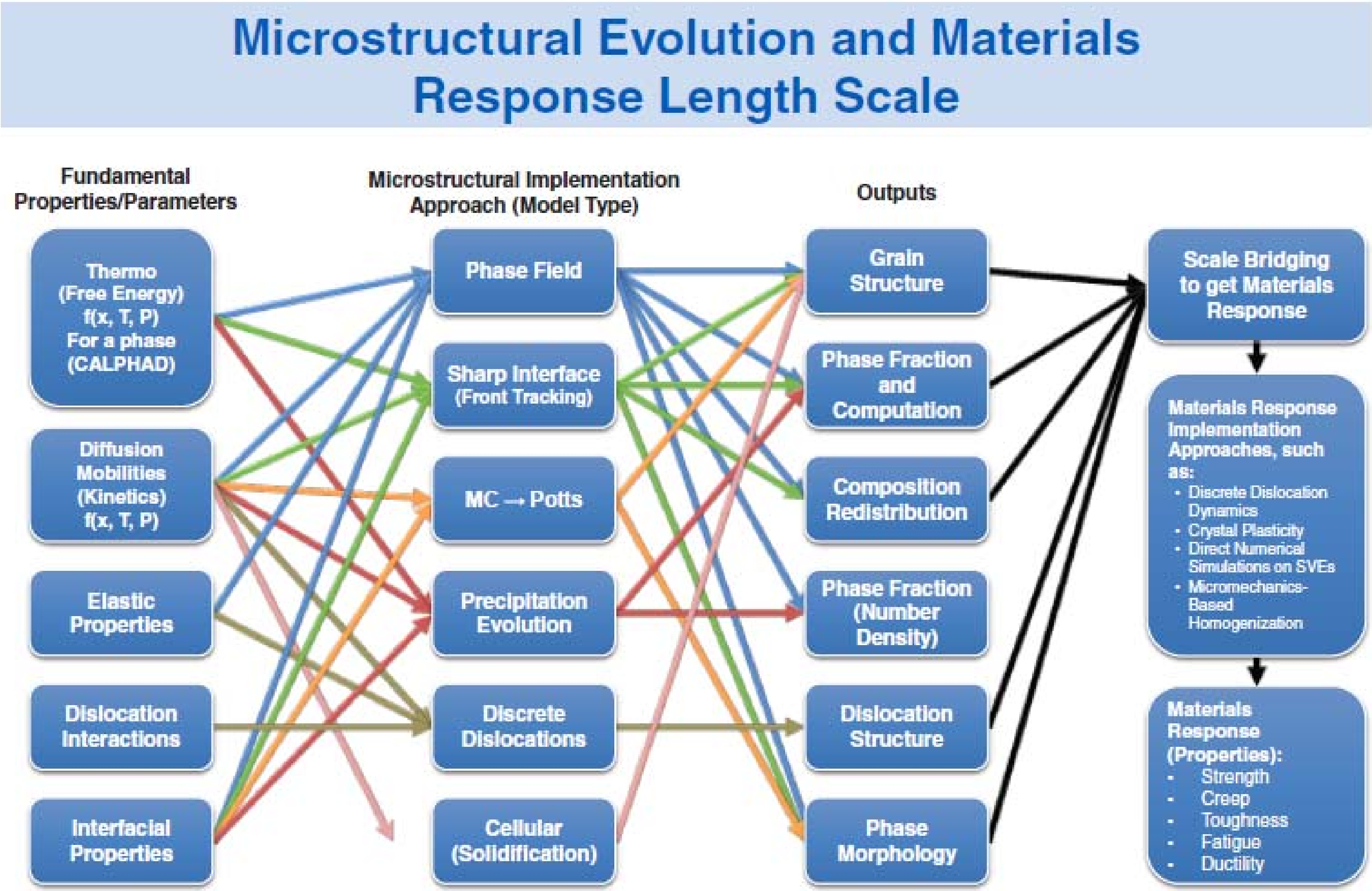


- Structure as in microstructure
  - Spatial distribution of structural features
    - Phases (with different compositions)
    - Grains (of different orientations)
    - Domains with different properties (electrical, magnetic etc.)





Mesoscale modelling (nm-µm)

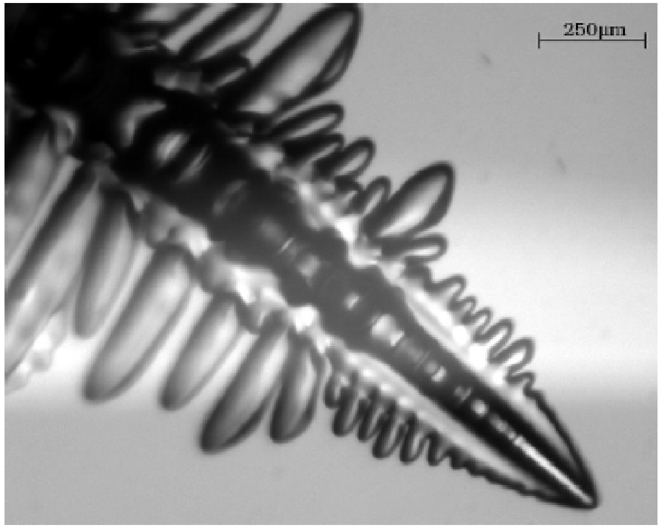


When should we consider the PFM?

- Modelling of moving interfaces

- Modelling microstructure evolution during phase transformations

- Effect of external stress, strain, transformation strain, anisotropic properties and complex morphologies



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Engineering problems suitable for the PFM

- Sintering (wetting and redistribution of alloy elements)
  - -ceramics
  - -sintered steels
  - -cemented carbides
- Soldering, brazing (wetting)
- Grain growth (lowers strength)
- Precipitation/dissolution (strength -homogenisation)
- Coarsening of precipitates (lowers strength)
- Spinodal decomposition (e.g. 475°C-embrittlement in steels, strengthening of cemented carbides))
- Martensite formation

PFM – the importance of interfaces

- The PFM is a diffuse interface method
  - Compare with DICTRA and TC-PRISMA, which are sharp interface methods
- Conditions at the interface
  - Local equilibrium assumption (DICTRA and TC-PRISMA, but not for the PFM)

Sharp vs. diffuse interface modelling of phase transformations

- **Sharp:**

\+ Easy to program, well-defined interface position

\- Conditions at the interface

Can be cumbersome in higher dimensions and for complex shapes

- **Diffuse (phase-field):**

\+ Easily extended to 3D

No explicit tracking of interfaces

No need to specify conditions at the interface

Good for complex shapes

\- Often computationally demanding

Often requires mesh adaptivity

Basics of the PFM I

- The microstructure is described with a number of phase field variables e.g.
  - Concentration
  - Crystal structure
  - …
- Time evolution of the field variables from partial differential equations (PDEs)
  - Cahn-Hilliard equation
  - Allen-Cahn equation
- No explicit tracking of the moving interfaces

Basics of the PFM II

- The concept of an order parameter (often denoted by η or ϕ)

Parameters that characterizes the variations in state during a phase transformation e.g. site fraction and magnetization, Bain variants etc.

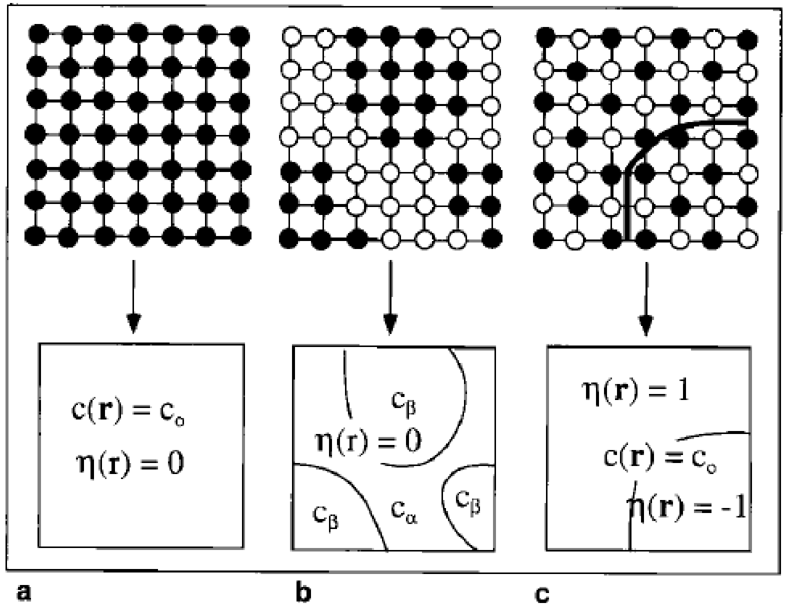

Figure 1. Schematics demonstrating the representation of morphologies by field variables. (a) disordered single phase, (b) two-phase mixture, and (c) ordered single phase.

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Table I. Examples of the Field Model Applications

Types of Processes	Field Variables
Isostructural Spinodal Decomposition	c
Ordering and Antiphase Domain Coarsening	η
Solidification in Single-Component Systems	η
180° Ferroelectric Domain Formation	P (polarization)
Solidification in Alloys	c, η
Precipitation of Ordered Intermetallics with	
Two Kinds of Ordered Domains	c, η
Four Kinds of Ordered Domains	$c, \eta_1, \eta_2, \eta_3$
90° Ferroelectric Domain Formation	P_1, P_2, P_3
Cubic→Tetragonal Displacive Transformation or Martensitic Transformation	η_1, η_2, η_3
Tetragonal Precipitates in a Cubic Matrix	$c, \eta_1, \eta_2, \eta_3$
Ordered Precipitate Morphology under Stress	$c, \eta_1, \eta_2, \eta_3$
Grain Growth in a Single-Phase Material	$\eta_1, \eta_2, \ldots, \eta_Q$
Grain Growth in a Two-Phase Mixture	$c, \eta_1, \eta_2, \ldots, \eta_Q$

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Short history of the PFM I

- The name ”phase-field” – Fix 1983 (free boundary problems)
- Studies on solidification of pure melts – Langer 1980’s, Kobayashi’s dendrites 1990’s
- Van der Waals 1893: interfaces between liquids and solids (continuous variation of the density with an extra term $(\nabla\rho)^2$)

Short history of the PFM II

- 1956-58: Cahn and Hilliard and Hillert
  - Extra term $(\nabla c)^2$, ”gradient energy”
  - Equilibrium from variational analysis.
  - Dynamics from a diffusion equation derived from the total free energy. => **Cahn-Hilliard equation**

- 1979: Allen and Cahn, migration of APB, change in order parameter η (non-conserved).
  - Dynamics from a postulated equation derived from total free energy.
  - Similar equation postulated by Ginzburg-Landau in the 1950’s to represent superconductivity transformation.
  - => **AC/GL-equation (Allen-Cahn/Ginzburg-Landau)**

Kobayashi’s dendrites

Gordon Research Conference 1990’s

Physica D 63 (1993) 410–423
North-Holland

PHYSICA D

Modeling and numerical simulations of dendritic crystal growth

Ryo Kobayashi
Department of Applied Mathematics and Informatics, Ryukoku University, Seta, Ohtsu 520-21, Japan

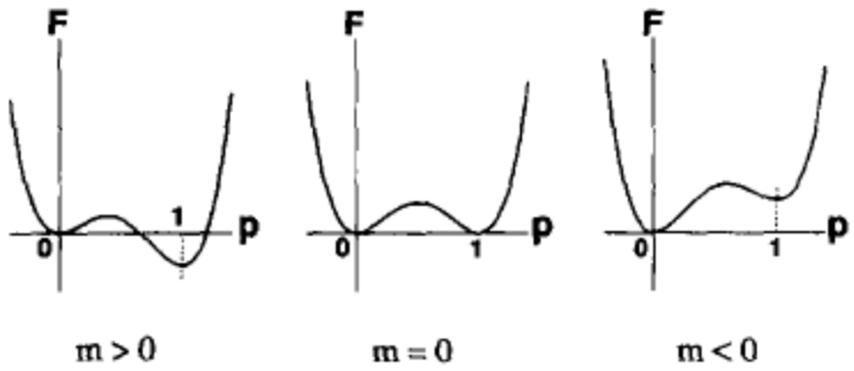
$$\tau\dot{\phi}=\varepsilon\nabla^2\phi+\gamma\phi(1-\phi)(\phi-\frac{1}{2}+m(T_m-T))$$

$$\dot{T}`=\nabla(\lambda_T\nabla T)+\frac{L}{c_p}\dot{\phi}$$

$$f=\frac{1}{2}\varepsilon(\nabla\phi)^2+\frac{\gamma}{4}\phi^2(1-\phi)^2-L\frac{T_m-T}{T_m}6(\frac{\phi^2}{2}-\frac{\phi^3}{3})$$

Solid $\phi=1$

Liquid $\phi=0$



Mathematics of the PFM

The total Gibbs energy:

$$G = \int_{\Omega} \left(G_m(\phi, x_k)/V_m + \frac{\varepsilon^2}{2} |\nabla \phi|^2 + \frac{\kappa^2}{2} |\nabla x_k|^2 \right) d\Omega$$

At equilibrium G is minimal, for fixed over-all composition. From variational calculus:

$$\frac{\delta G}{\delta \phi} = \left(\frac{\partial (G_m / V_m)}{\partial \phi} - \varepsilon^2 \nabla^2 \phi \right)$$

$$\frac{\delta G}{\delta x_k} = \frac{\partial (G_m / V_m)}{\partial x_k} - \kappa^2 \nabla^2 x_k$$

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Variational calculus

$$I = \int F(y, y', x)\,dx$$

Functional

$$\frac{\delta I}{\delta x}$$

Variational derivative

$$\frac{\delta I}{\delta x} = \frac{\partial F}{\partial y} - \frac{d}{dx}\left(\frac{\partial F}{\partial y'}\right)$$

Euler-Lagrange equation

Rate equations

$$J_k = -\sum L_{kj} \nabla \left(\frac{\delta G_m}{\delta x_j} \right)$$

Cahn-Hilliard Equation: ”Model B”

$$\dot{x}_k = \nabla \cdot \left[\sum L_{kj} \nabla \left(\frac{\partial G_m}{\partial x_j} - V_m \kappa_j^2 \nabla^2 x_j \right) \right]$$

AC/GL-equation: ”Model A”

$$\dot{\phi} = -M_\phi \frac{\delta G}{\delta \phi} = -M_\phi \left(\frac{\partial G_m / V_m}{\partial \phi} - \varepsilon^2 \nabla^2 \phi \right)$$

Modelling with the PFM I

Consider a binary two-phase system

How should we represent $G_m(x_i,\phi)$?

Wheeler, Boettinger and McFadden (WBM)

$$G_m(x_1,x_2,\phi)=(1-p(\phi))G_m^{\alpha}(x_1,x_2)+p(\phi)G_m^{\beta}(x_1,x_2)+g(\phi)W$$

Steinbach et al. Multi-Phase-Field (MPF)

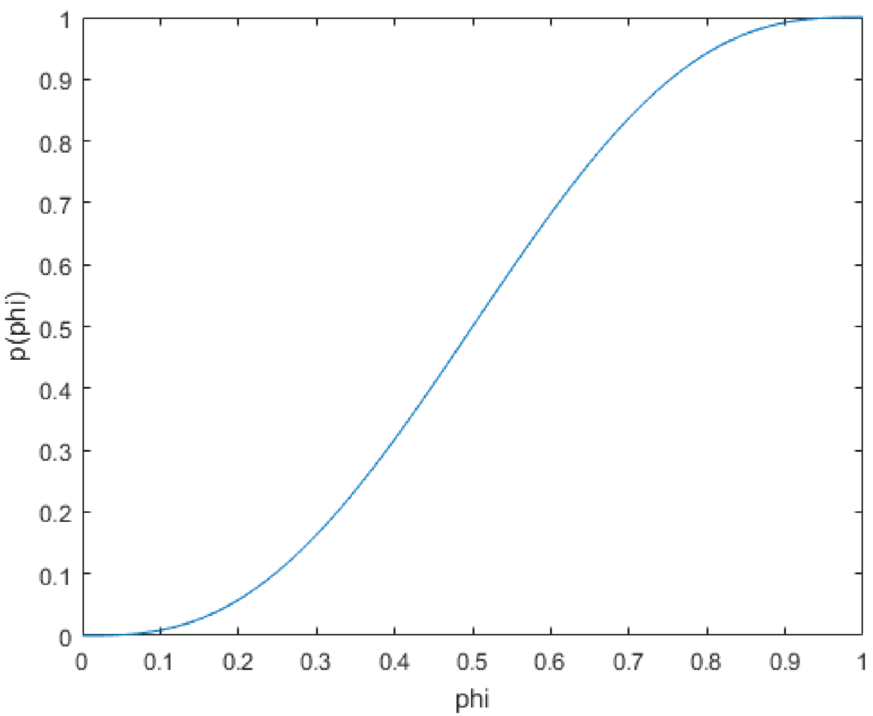
$$G_m(x_i,\phi)=(1-p(\phi))G_m^{\alpha}(x_1^{\alpha},x_2^{\alpha})+p(\phi)G_m^{\beta}(x_1^{\beta},x_2^{\beta})+g(\phi)W$$

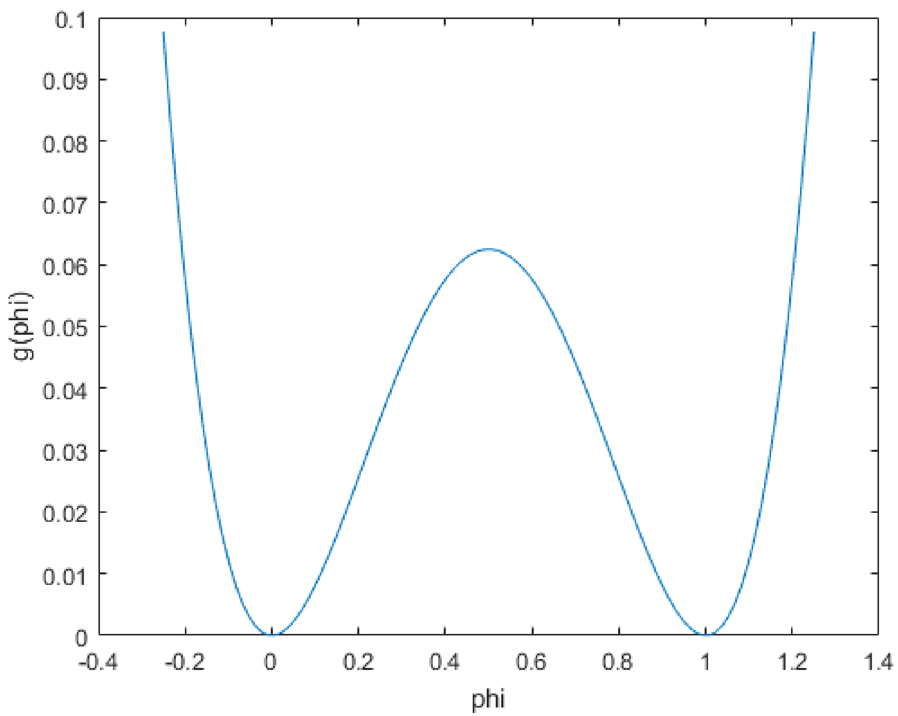
Modelling with the PFM II

Example polynomials

$$p(\phi) = \phi^3(10 - 15\phi + 6\phi^2)$$

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





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Examples of applications

- Martensite formation in Fe-C
- Spinodal decomposition in Fe-Cr alloys
- Sigma phase formation in a duplex stainless steel

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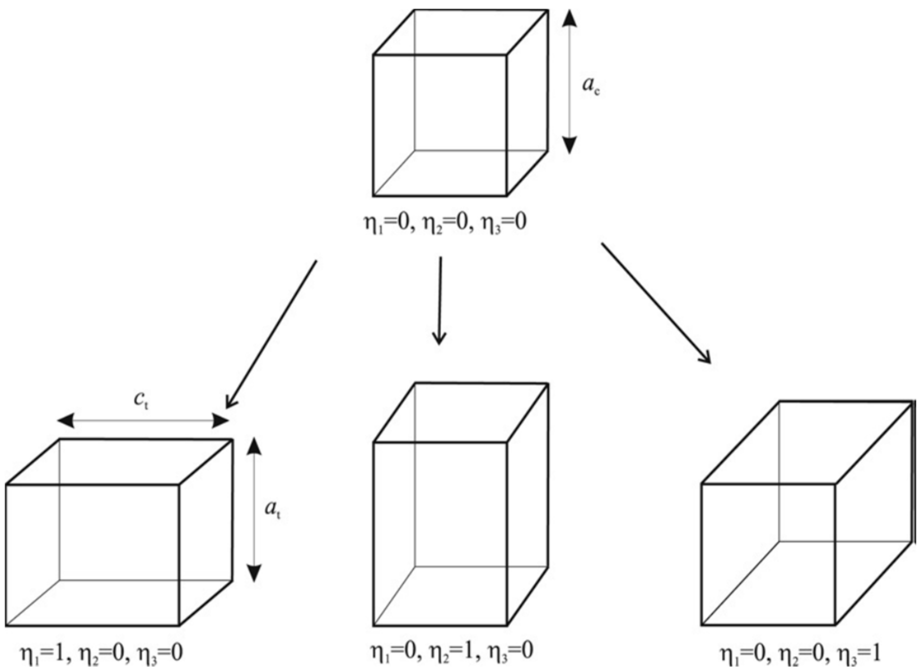
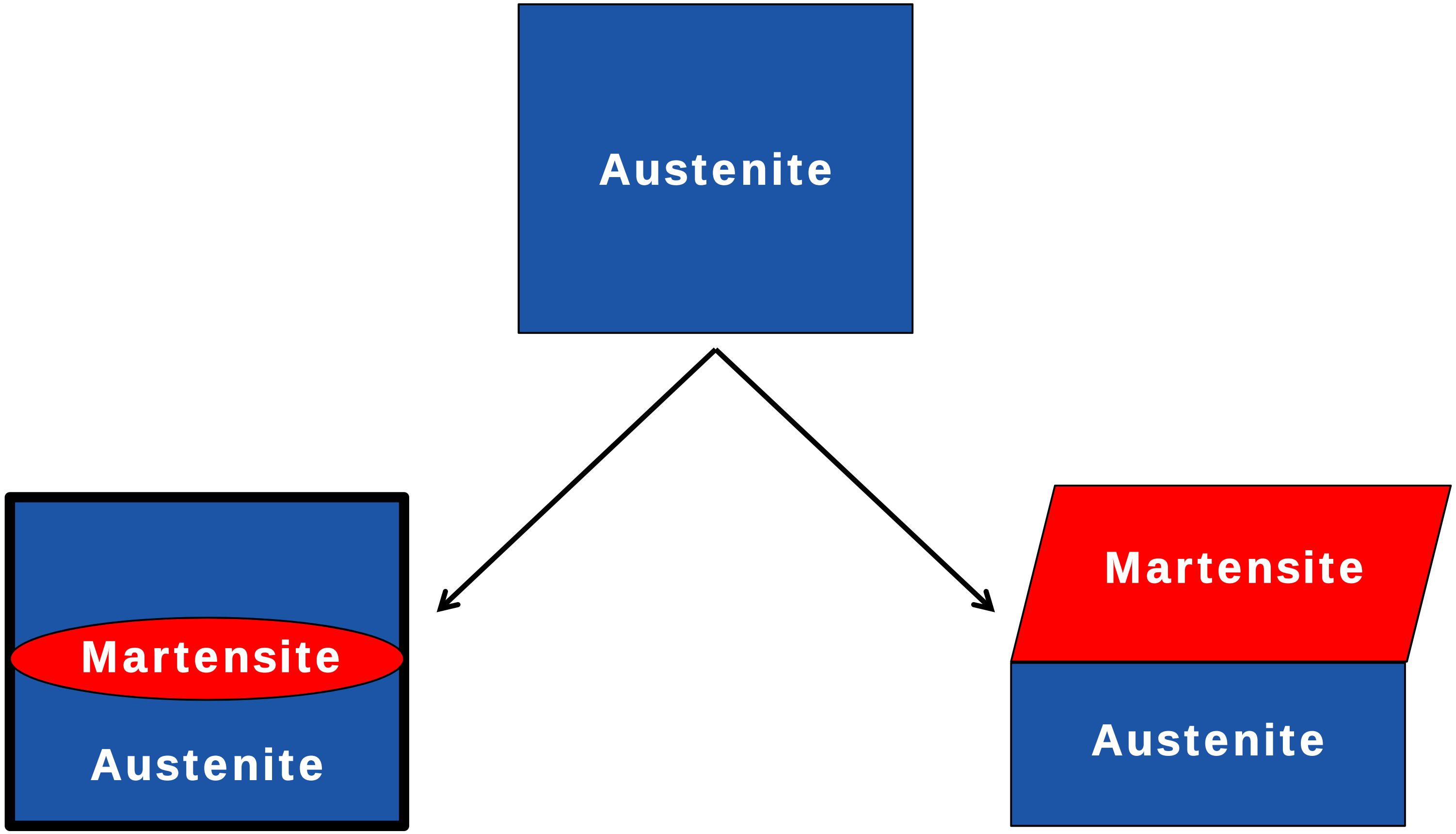
Martensite formation in Fe-C

- MT is diffusionless, i.e. no variation in concentration
- Phase field Equation: $$\frac{\partial \eta_p}{\partial t} = -\sum_{p=1}^{p=v} L_{pq} \frac{\delta G}{\delta \eta_p}$$ (Allen-Cahn)
- L_{pq} : Kinetic coefficient, corresponds to interface mobility
- Phase field variable: η_p : (η_1 , η_2 , η_3)
- **$G = G_{chemical} + G_{gradient} + G_{elastic} + G_{plastic}$**



One Allen-Cahn type equation for each Bain variant

Shape of Martensite...



Constrained
(Zero displacement BC)

Unconstrained
(Stress free BC)

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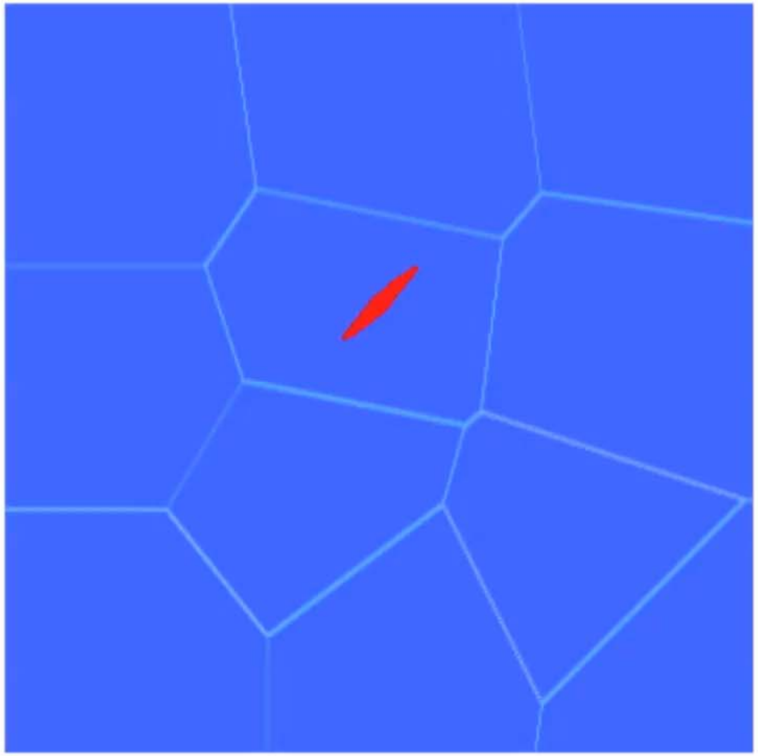
Simulation parameters

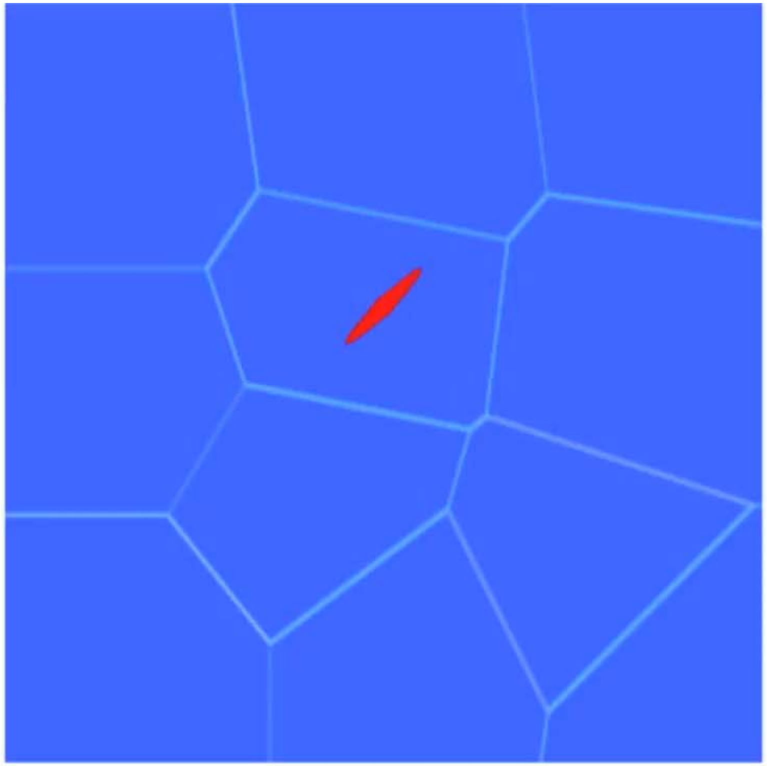
- Fe-0.3C alloy
- Physical size of the system: 1μm
- M_s temperature (Experimental value)
- Driving force calculated from Thermo-Calc at M_s
- Bain strains (ε^T) calculated from Lattice constants (Experimental)
- Isotropic Elasticity case : E = 200 GPa
- Anisotropic Elastic modulii(**c**): Experimental values

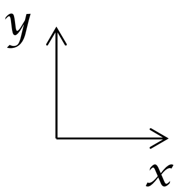
Martensite formation in Fe-C: 2D simulation

Zero displacement BC

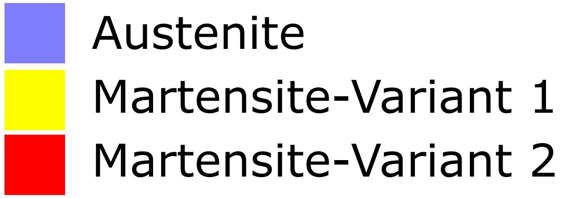


Stress free BC





Malik et al.



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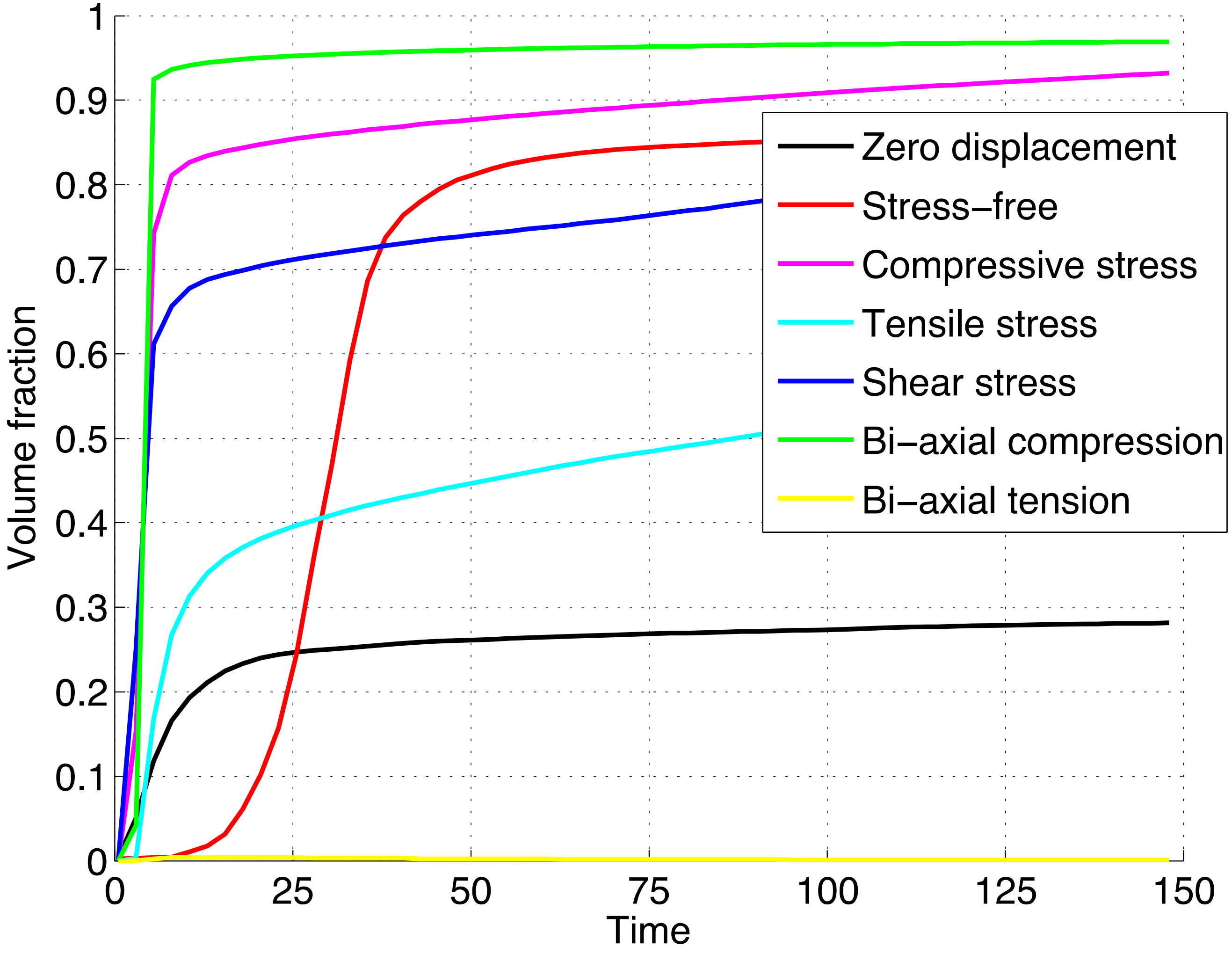
Results from 2D simulations



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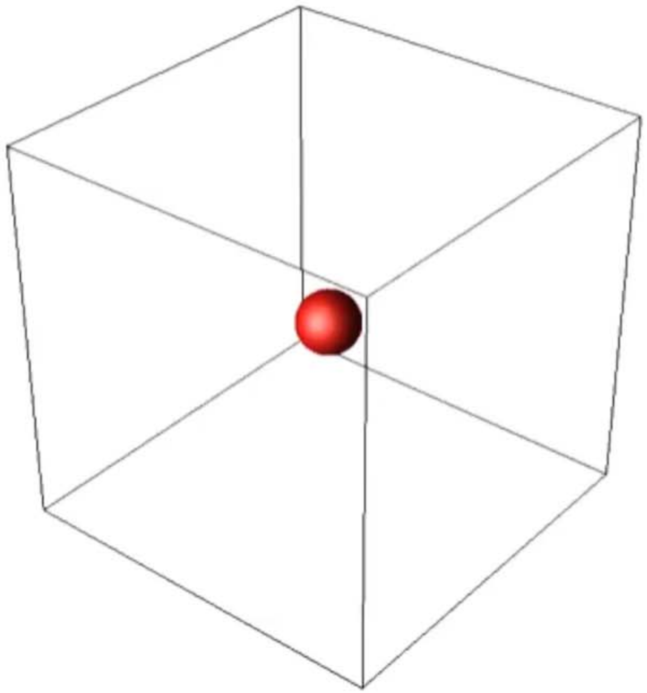
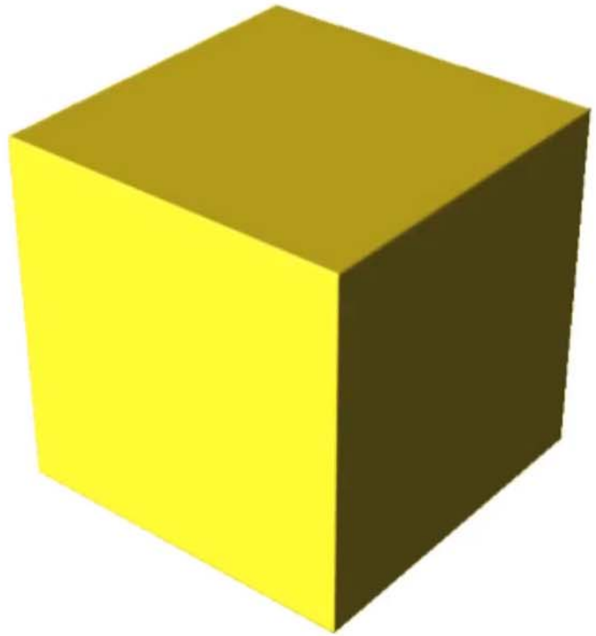
Martensite formation in Fe-C: 3D simulation

Zero displacement BC



Stress free BC



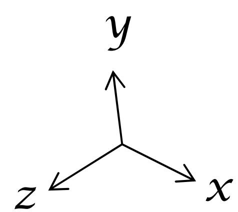
Austenite

Martensite-V1

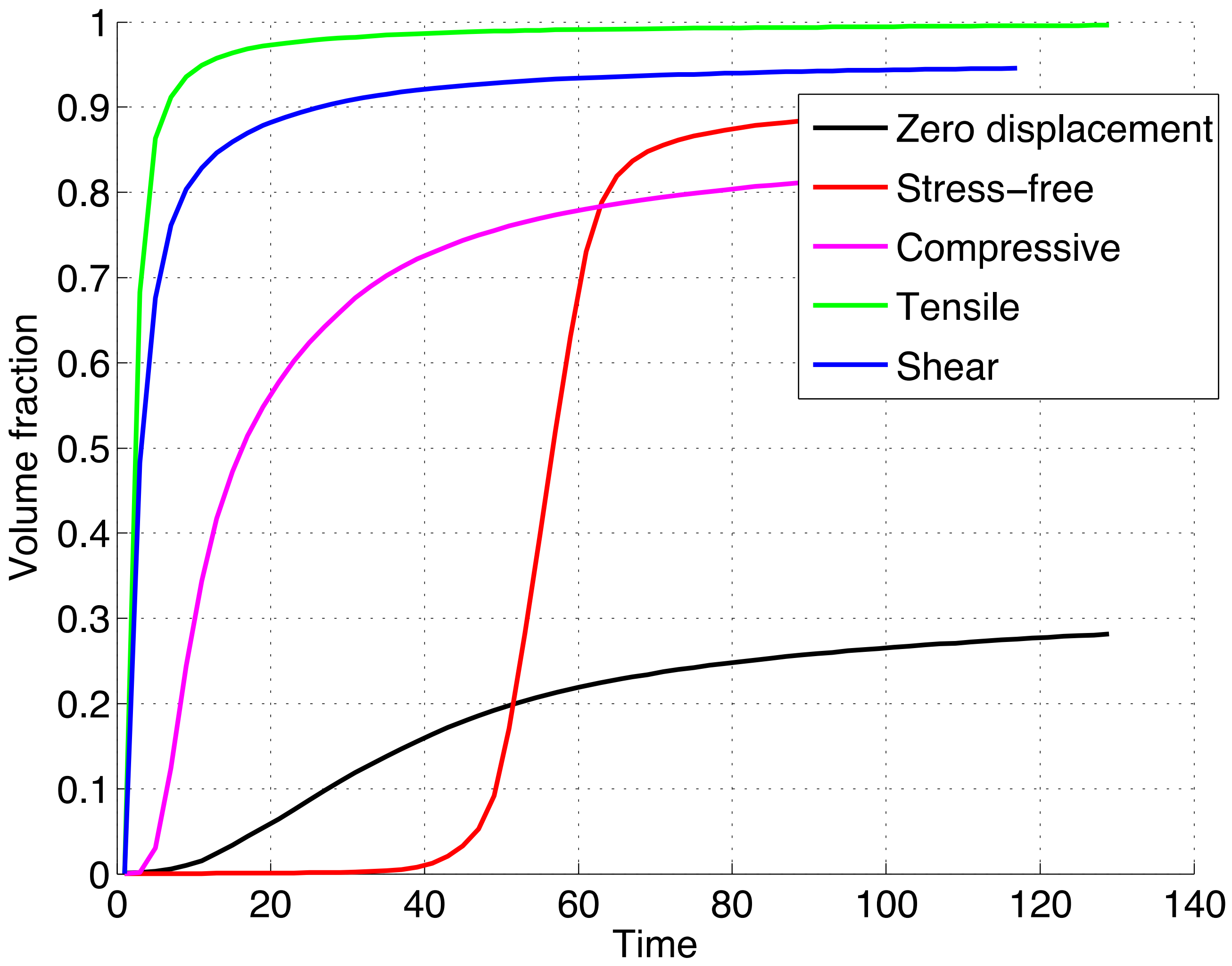
Martensite-V2

Martensite-V3

Malik et al.



Results from 3D simulations



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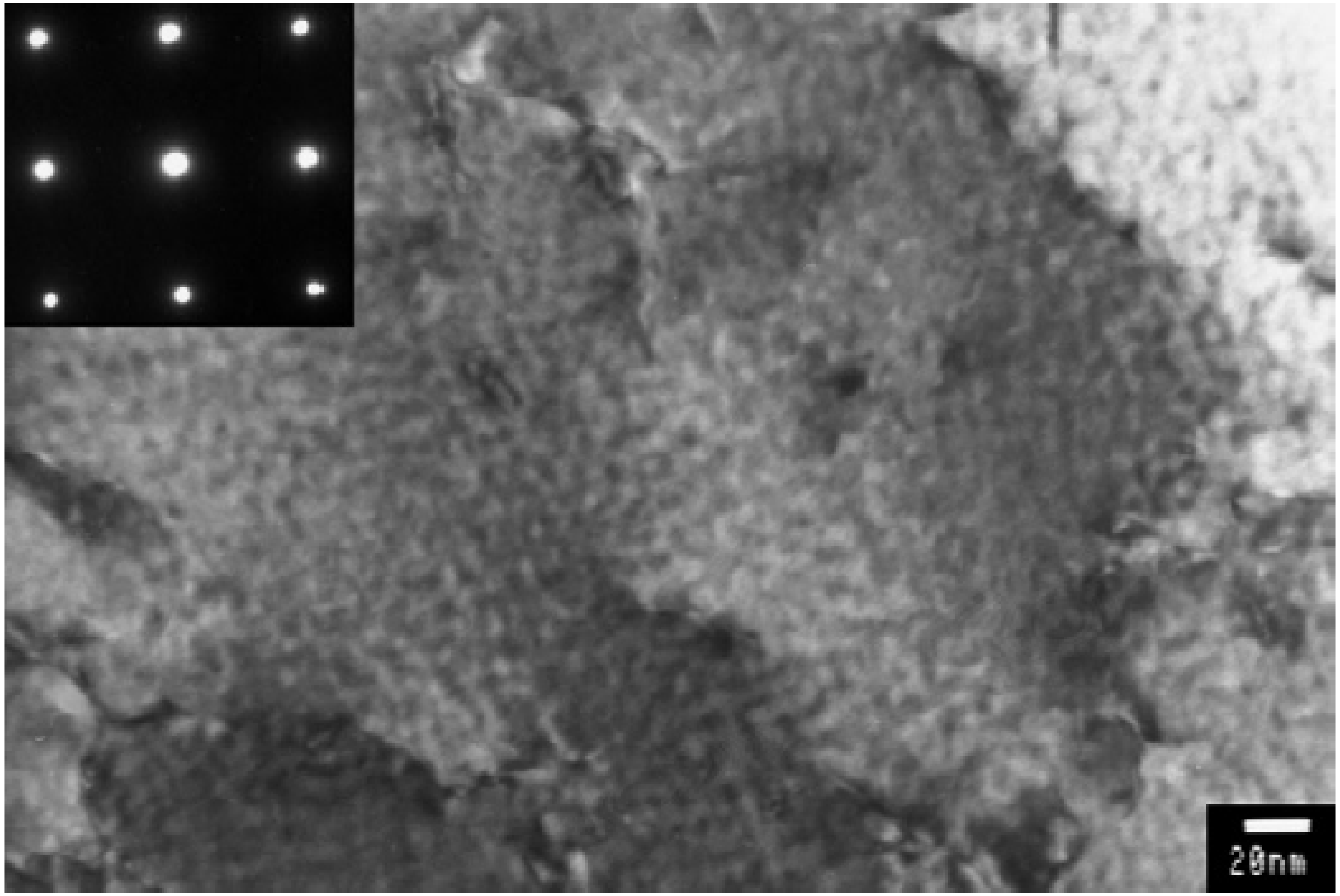
Conclusions

- 3D simulations are required to investigate the stress effects!
- In a Fe-0.3%C system:
  - Maximum volume fraction of the martensite phase can be achieved by applying the tensile stress.
  - Applying the compressive stress, reduces the volume fraction of the martensite phase.

Characteristic features of spinodal decomposition

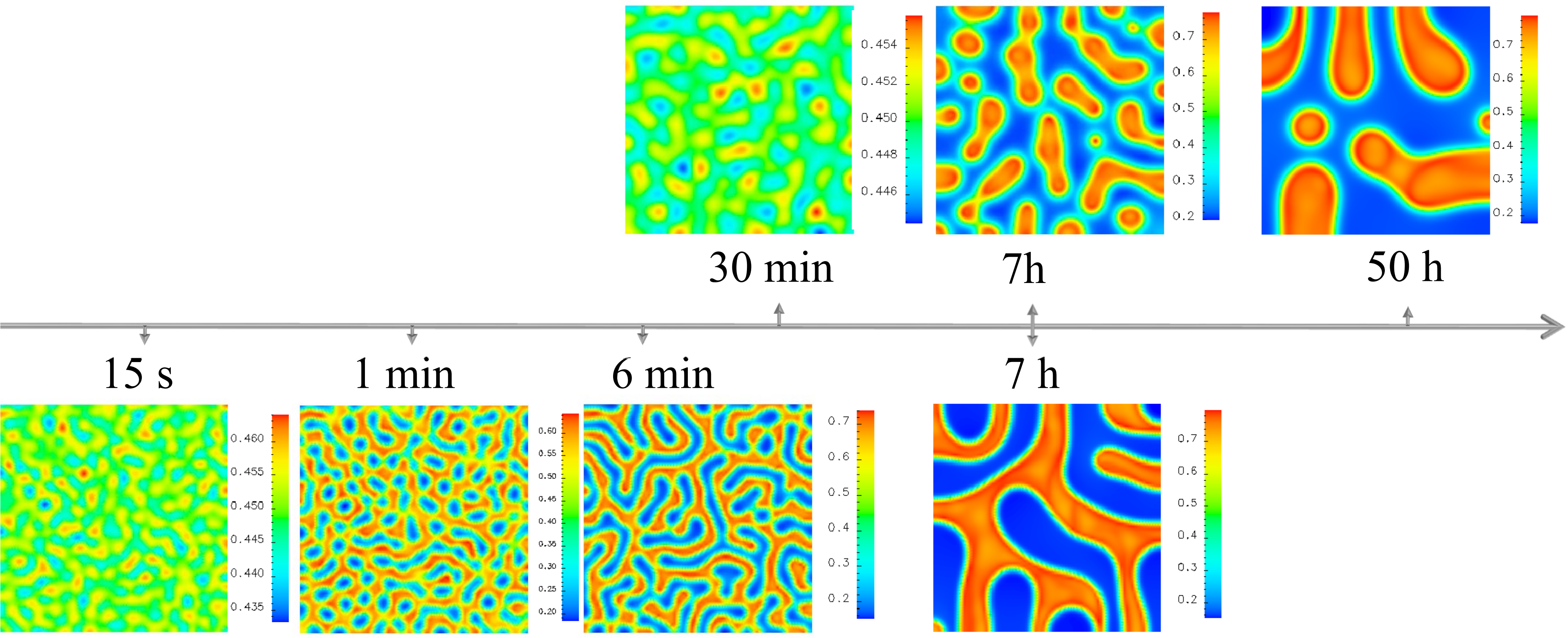
Modulated or mottled constrast in ferrite in a duplex stainless steel



Hättestrand et al.

Solving the Cahn-Hilliard equation: Simulation results for Fe-45at%Cr at 773K

Thermodynamics: Andersson and Sundman, 1987



Thermodynamics: Xiong et al., 2010

Sigma phase formation in a duplex stainless steel (Fe-25Cr-7Ni-4Mo)

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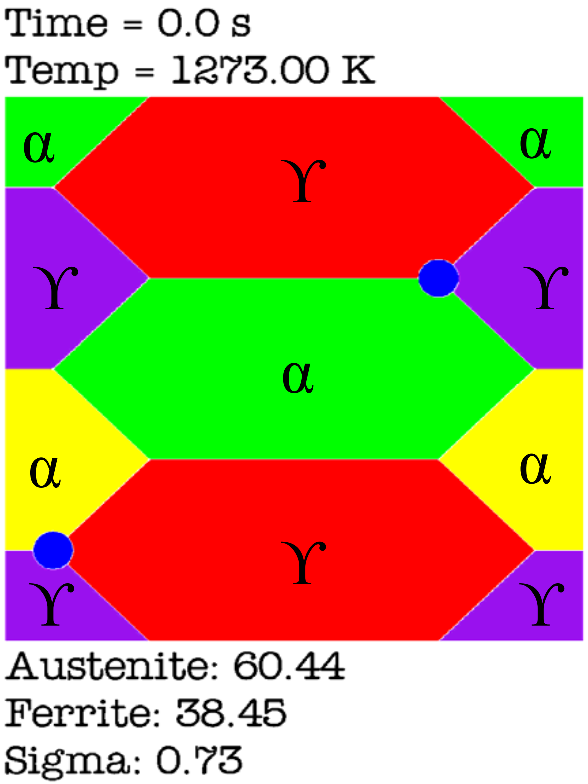
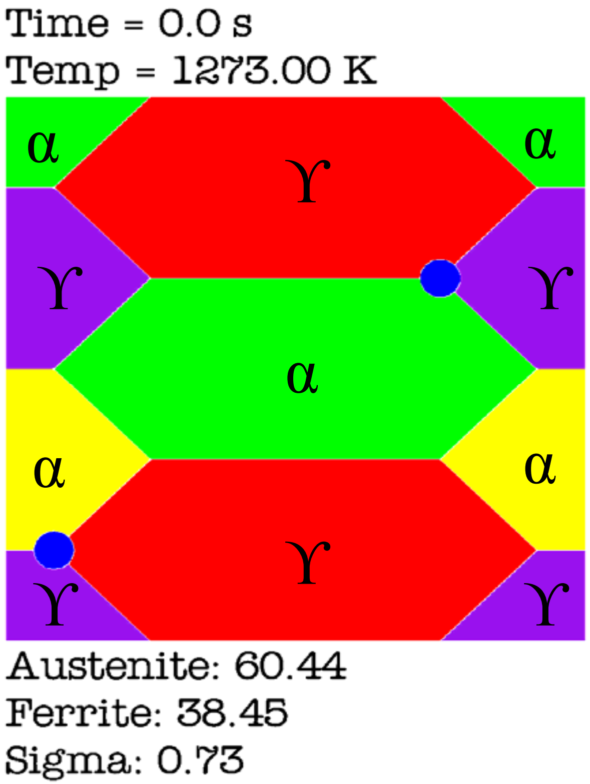
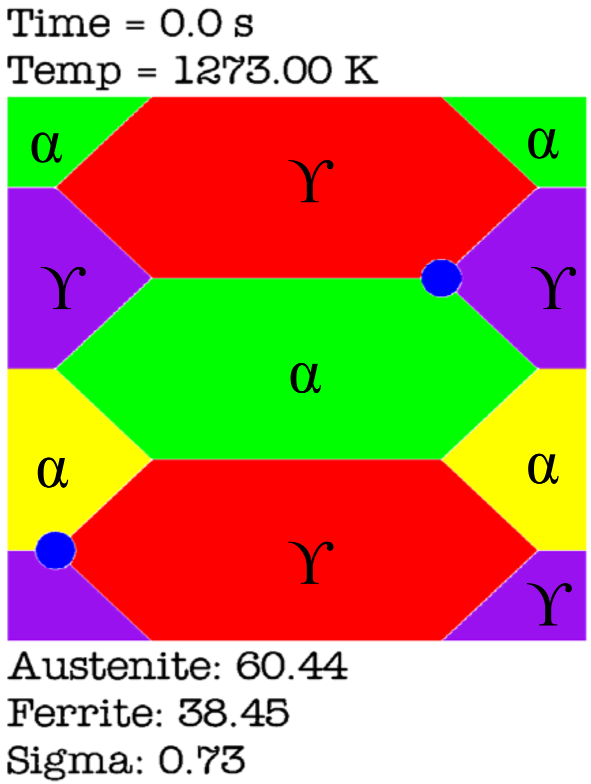
Continuous Cooling from 1273K to 950K



1K/s



50K/s



100K/s

Malik et al.

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Issues in phase-field modelling

- Computational efficiency
- Realistic length scales: interfaces thicknesess vs. size of grains/phase domains
- Number of domains/grains
- Nucleation
  - Evolution equations are deterministic i.e. explicit nucleation events cannot be handled with the original Cahn-Hilliard, Allen-Cahn equations

$$\frac{dG}{dt} \leq 0$$

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Codes for the PFM

- Most groups in the field have their own in-house code
- Many open source codes available for solving PDEs
  - femLego (https://www.mech.kth.se/~minh/femLegoPar/introduction.htm)
  - FiPy (http://www.ctcms.nist.gov/fipy/)
  - Moose (http://mooseframework.org/)
  - OpenPhase (http://www.openphase.de/)
  - …
- One commercial code: MICRESS (http://web.micress.de/)

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The home assignment

- Implement WBM and MPF for a binary, two-phase system using e.g. Matlab

- Perform numerical experiments

- Discussion of the home assignment Friday May 12, 9-10 (Efim Borukhovich)