12th ALEMI workshop

Phase-field model for mixed mode transformations and its perspective for steel

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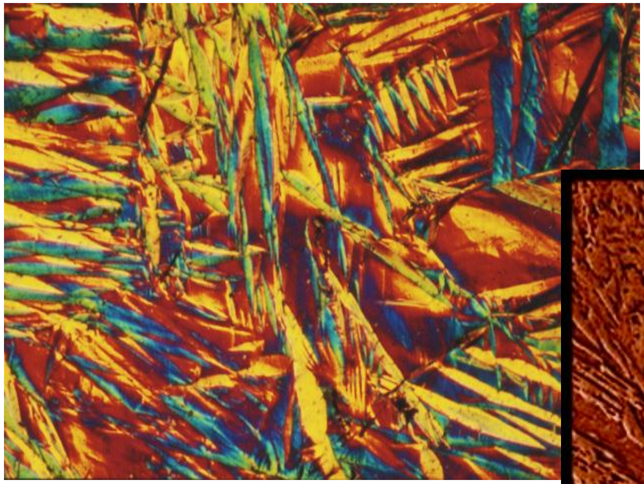
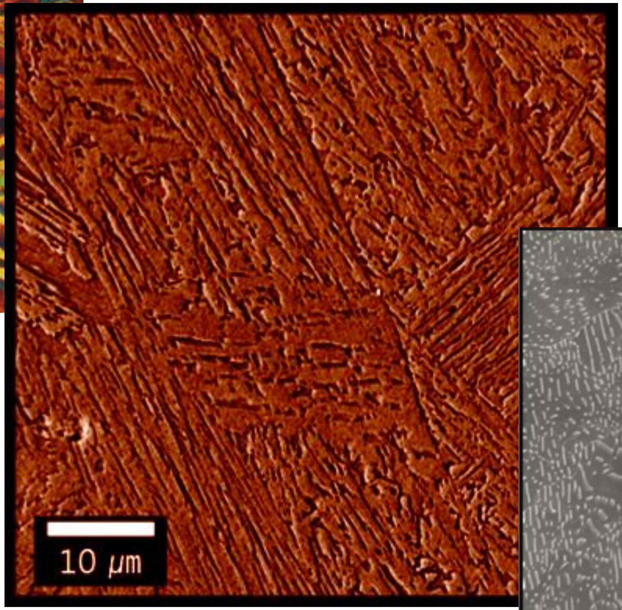
Steel Microstructures

Martensite



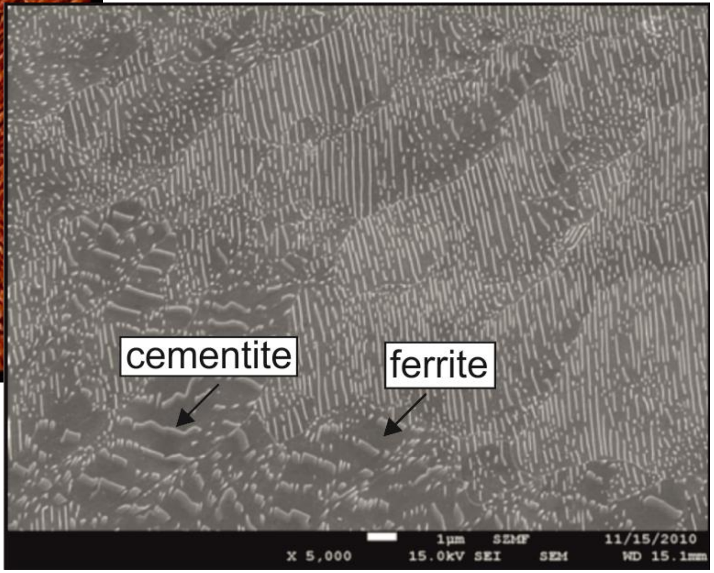
from lecture material
of H.K.D.H.Bhadeshia

Bainite



Junhak Pak, Dong Woo Suh,
and H. K. D. H. Bhadeshia,
Scripta Materialia 66 (2012)

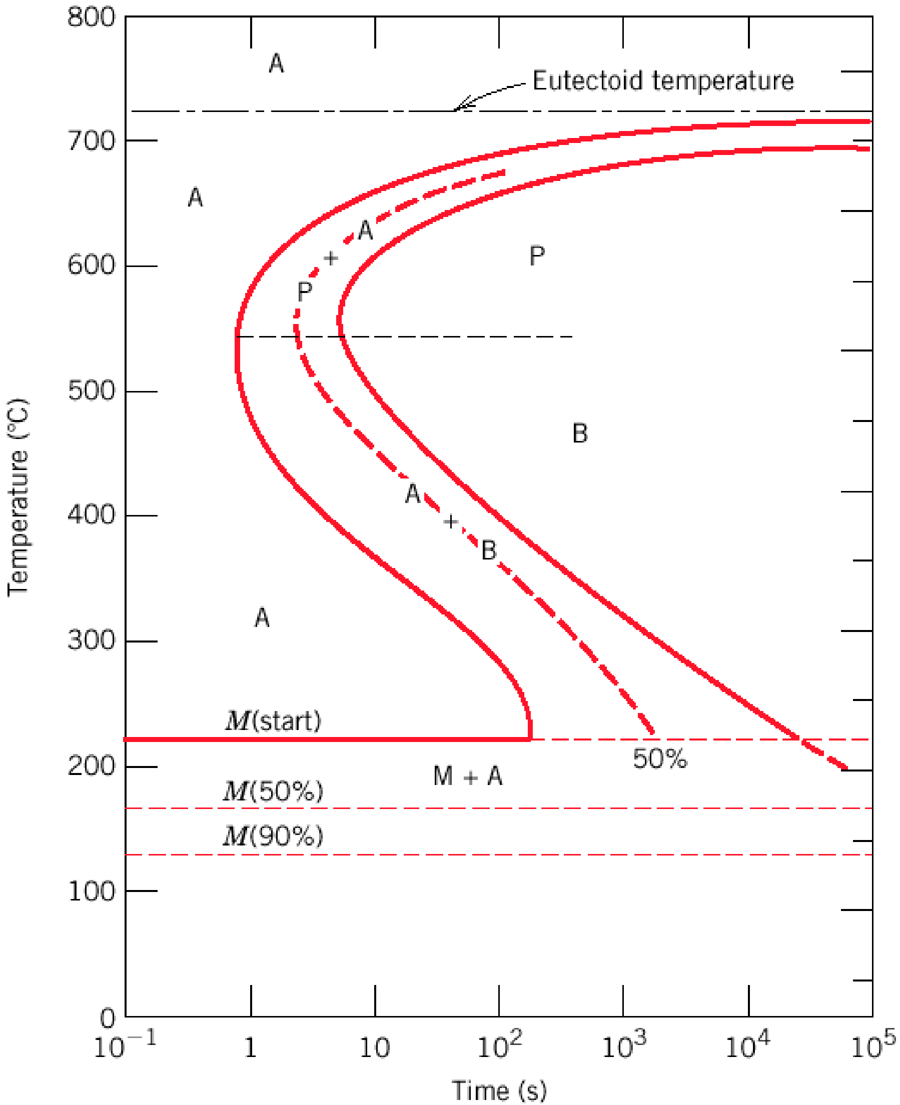
Pearlite



28Mn6 steel Benteler Stahl/Rohr “as-cast” microstructure

Steel forms many phases and microstructures
and every microstructure posses different properties!

Fe-C TTT Diagram



The key to steel properties are highly non-equilibrium phase transformations (e.g. martensitic, bainitic, …)

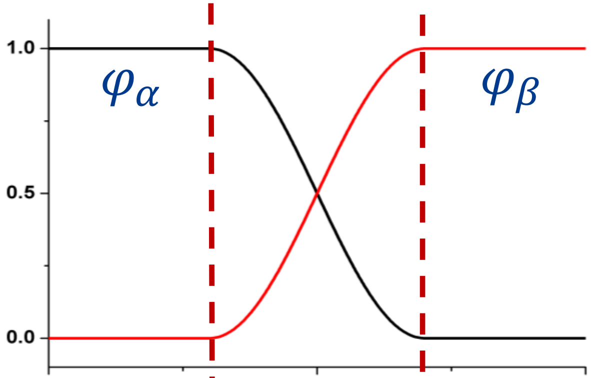
Outline

1. Standard multi phase field model
2. Phase field model for non-equilibrium transformations
3. Modeling phase transformations in steel
4. New developments
5. Summary

Phase field, properties and free energy

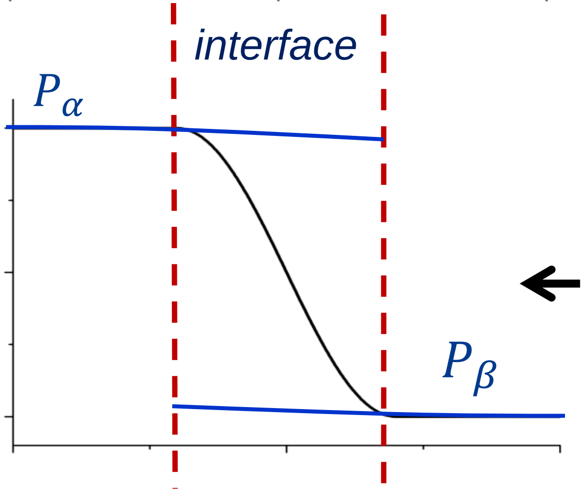
interfacial chemical elastic disl. dens.

$$F = \int_{\Omega} f^{GB} + f^{CH} + f^{EL} + f^{DD} + \cdots$$



Phase field

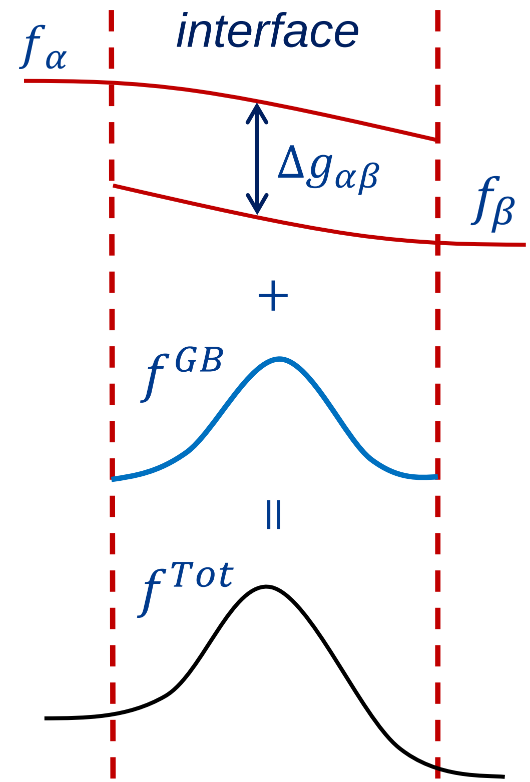
$$\boxed{\varphi_\alpha + \varphi_\beta \equiv 1}$$



Properties

$$\boxed{P = \varphi_\alpha * P_\alpha + \varphi_\beta * P_\beta}$$

Energy



Free energy densities and evolution equations

Interfacial energy density

$$f^{GB} = \sum_{\alpha,\beta=1}^{N} \frac{4\sigma_{\alpha\beta}}{\eta_{\alpha\beta}} \left\{ \frac{\eta^2_{\alpha\beta}}{\pi^2} \left|\nabla\phi_\alpha\right| \cdot \left|\nabla\phi_\beta\right| + \phi_\alpha\phi_\beta \right\}$$

Phase field equation

$$\dot{\phi}_\alpha + \vec{u}_\alpha \cdot \nabla\phi_\alpha = -\sum_{\beta=1}^{N} \frac{\mu_{\alpha\beta}}{N} \left(\frac{\delta F}{\delta\phi_\alpha} - \frac{\delta F}{\delta\phi_\beta} \right)$$

Chemical energy density

$$f^{CH} = \sum_{\alpha=1}^{N} \phi_\alpha f_\alpha(\vec{c}_\alpha) + \vec{\mu}\left(\vec{c} - \sum_{\alpha=1}^{N} \phi_\alpha \vec{c}_\alpha \right)$$

Advection-diffusion equation

$$\dot{\vec{c}} + \sum_{\alpha=1}^{N} \vec{u}_\alpha \cdot \nabla(\phi_\alpha \vec{c}_\alpha) = \nabla \cdot \left(\sum_{\alpha=1}^{N} M_\alpha \phi_\alpha \nabla \frac{\delta F}{\delta \vec{c}_\alpha} \right) + \nabla \cdot \vec{\vec{j}}_{at}$$

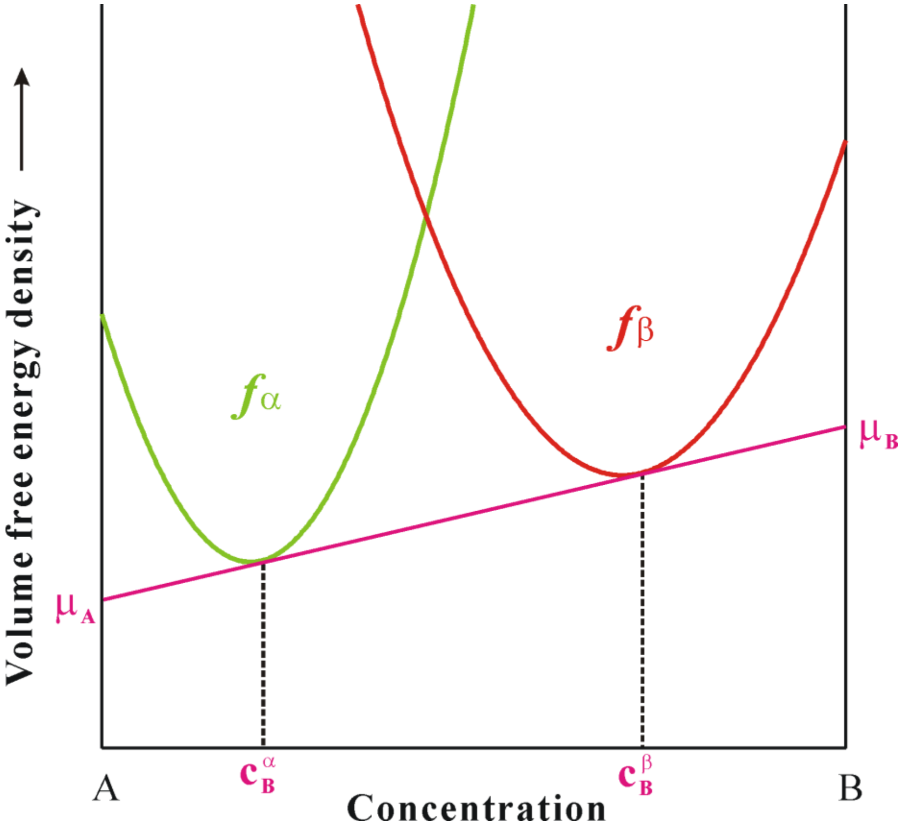
Elastic energy density

$$f^{EL} = \frac{1}{2} \sum_{\alpha=1}^{N} \phi_\alpha \left(\varepsilon^{ij}_\alpha - \varepsilon^{*ij}_\alpha \right) C^{ijkl}_\alpha \left(\varepsilon^{kl}_\alpha - \varepsilon^{*kl}_\alpha \right)$$

Elastic equilibrium equation

$$0^i = \nabla^j \sigma^{ij} = \nabla^j \frac{\delta F}{\delta \varepsilon^{ij}};$$

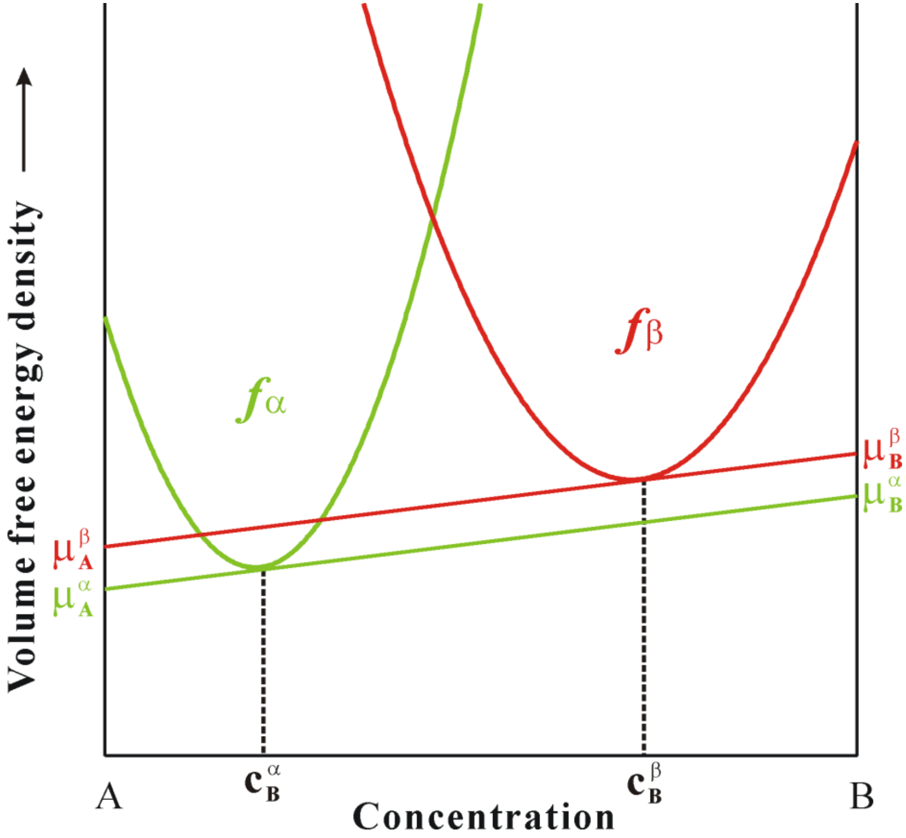
Current approaches: Local equilibrium



- Double tangent constraint
- Equilibrium concentrations
- Equal chemical potential

DICTRA

Current approaches: Quasi equilibrium



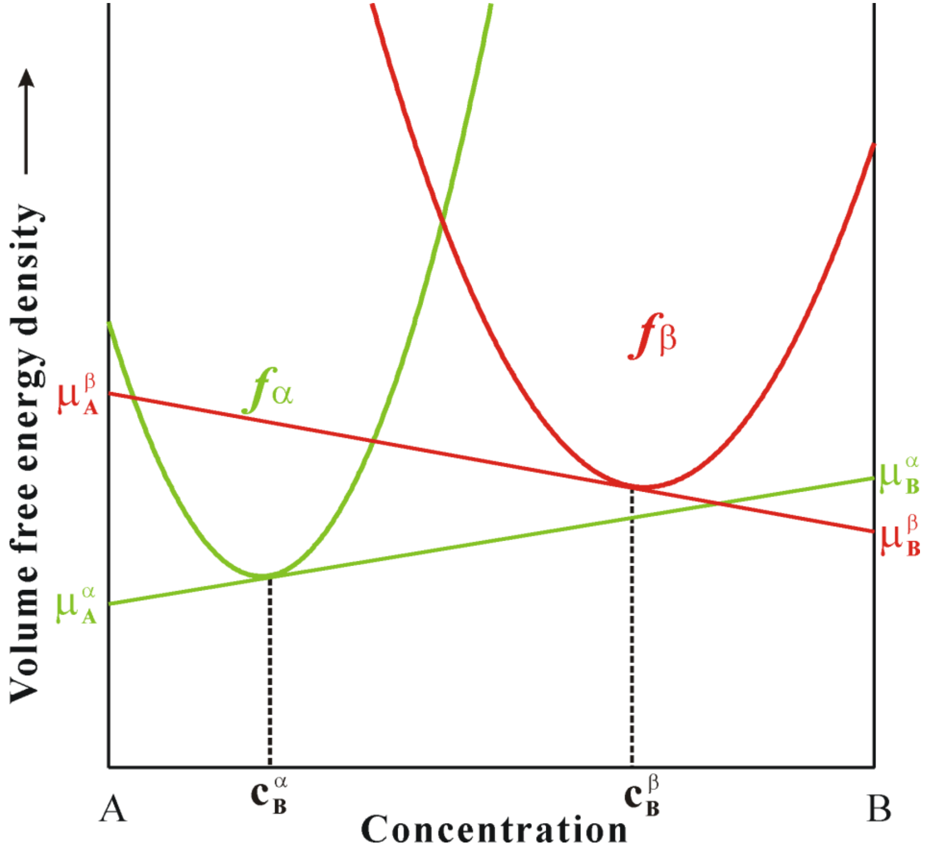
- Parallel tangent constraint
- Equal diffusion potential

$$\mu_\alpha = \frac{\partial f_\alpha(T, c_\alpha)}{\partial c_\alpha} = \mu_\beta = \frac{\partial f_\beta(T, c_\beta)}{\partial c_\beta} \equiv \mu$$

$$c(x,t) = c_\alpha(x,t)\phi(x,t) + c_\beta(x,t)[1 - \phi(x,t)]$$

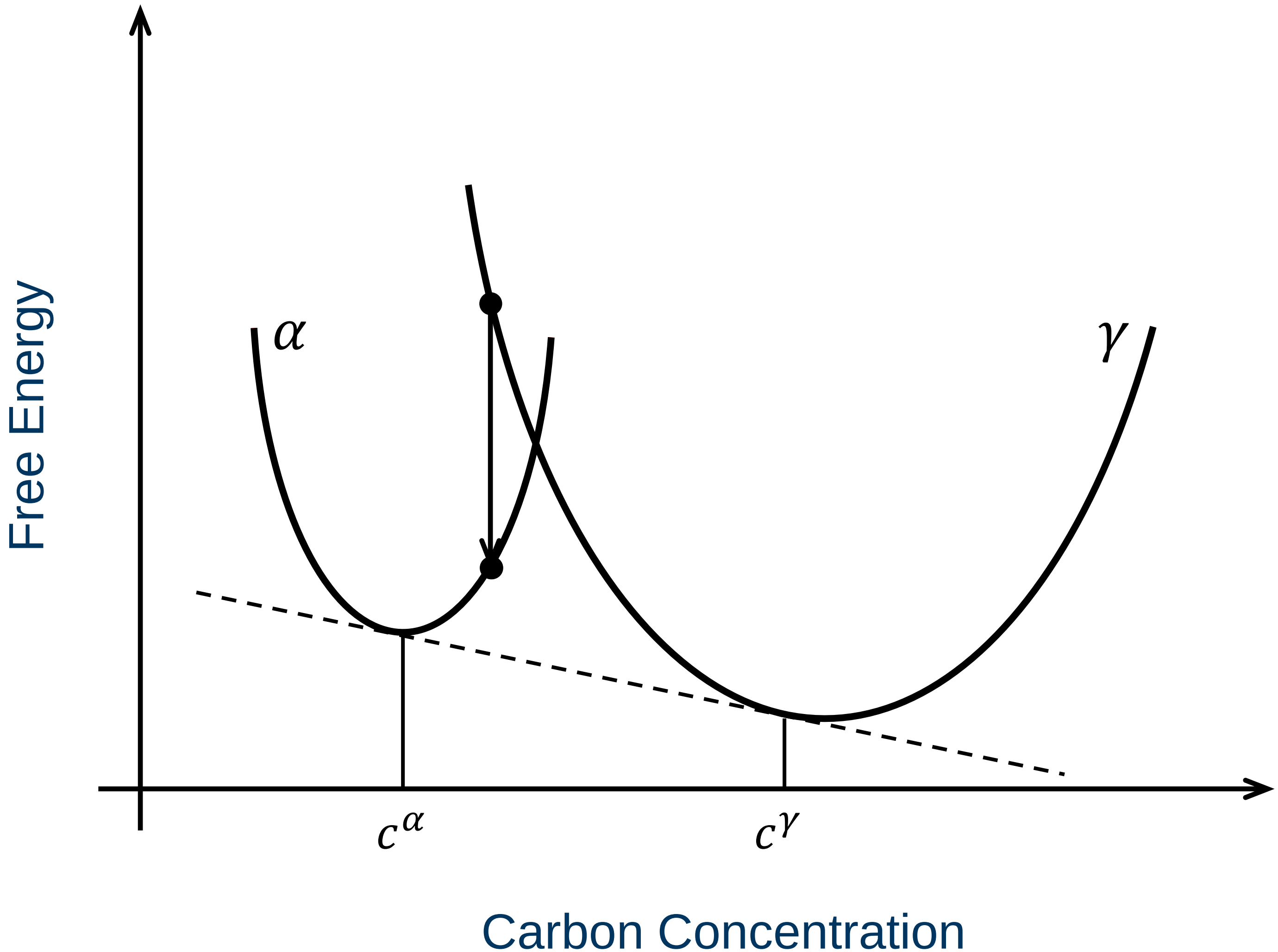
$$\dot{c} = \nabla D_\alpha \phi \nabla c_\alpha + \nabla D_\beta (1-\phi) \nabla c_\beta$$

The general case



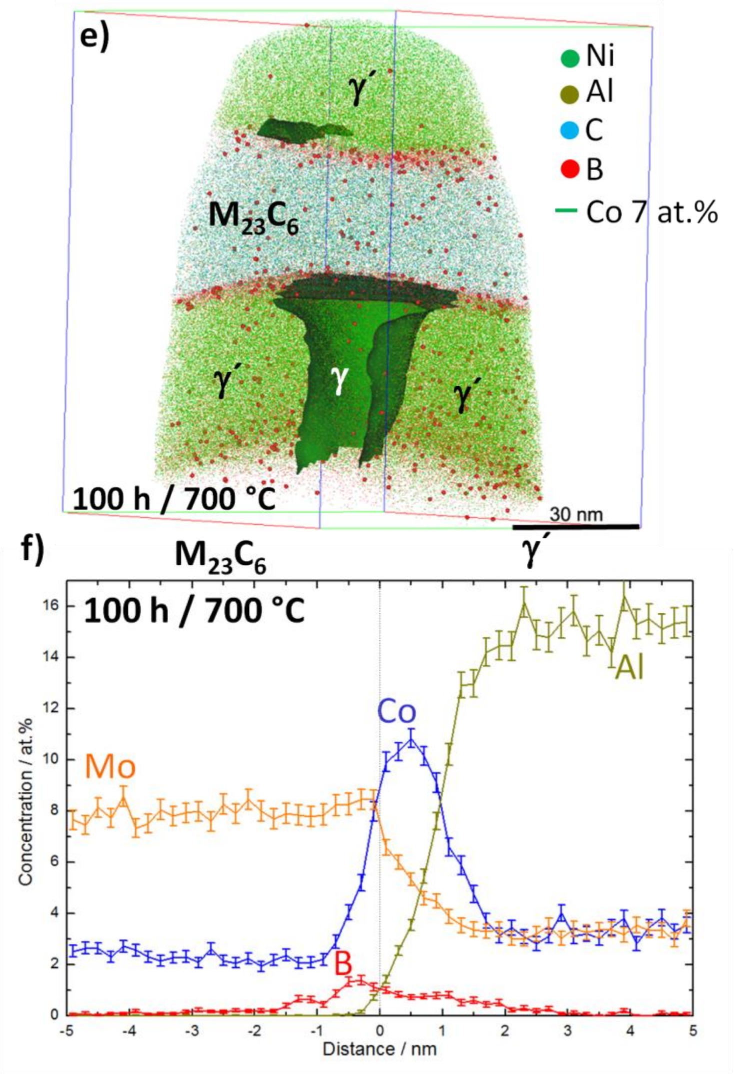
$$\mu_\alpha = \frac{\partial f_\alpha}{\partial c_\alpha} \neq \mu_\beta = \frac{\partial f_\beta}{\partial c_\beta} \neq \mu$$

Effect of stress



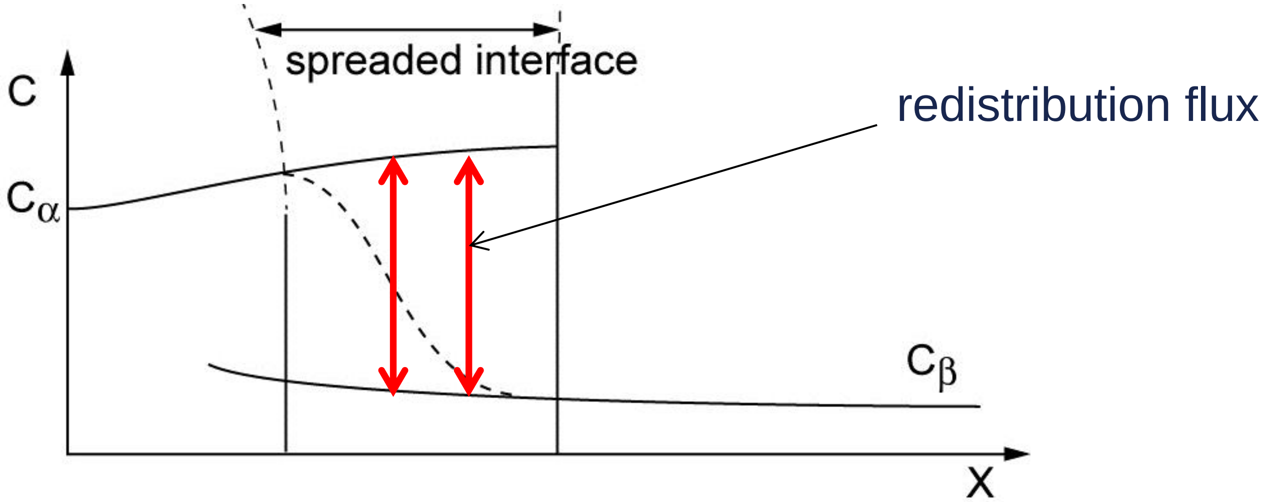
Coarse graining of the diffusion equation

$$\dot{c} = \vec{\nabla}\left(M(c,\phi)\frac{\partial^2 f}{\partial c^2}\ \vec{\nabla} c \right)$$



D. Tytko et. al, Acta Mat 2012

Coarse graining of the diffusion equation



$$\dot{c}_\alpha(\vec{x}) = -4\pi^2 M \int_{|\vec{k}|<k_0} k^2 \mu(\vec{k}) e^{-2\pi i \vec{k}\vec{x}} d\vec{k} + P(\mu_\beta - \mu_\alpha); \qquad \vec{x} \in \Omega_\alpha$$

$$\dot{c}_\beta(\vec{x}) = -4\pi^2 M \int_{|\vec{k}|<k_0} k^2 \mu(\vec{k}) e^{-2\pi i \vec{k}\vec{x}} d\vec{k} + P(\mu_\alpha - \mu_\beta); \qquad \vec{x} \in \Omega_\beta.$$

$$P = -\frac{1}{(\mu_\alpha - \mu_\beta)} 4\pi M \int_{|\vec{k}|<k_0} k^2 \mu(\vec{k}) e^{-2\pi i \vec{k}\vec{x}} d\vec{k}.$$

Diffusion equation in one phase

$$\phi_\alpha \dot{c}_\alpha = \vec{\nabla}\left(\phi_\alpha D_\alpha \vec{\nabla} c_\alpha\right) + P_{\alpha\beta}\phi_\alpha\phi_\beta\left(\tilde{\mu}_\beta - \tilde{\mu}_\alpha\right) + \phi_\alpha \dot{\phi}_\alpha (c_\alpha - c_\beta)$$

diffusion within one phase

redistribute solute if there is a chemical potential difference between the phases

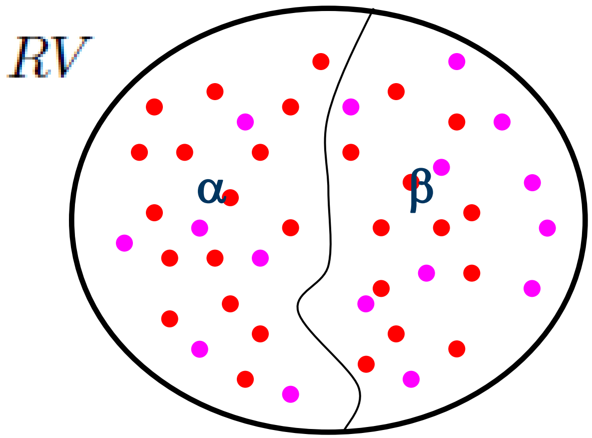
phase concentrations change if there is a phase change

Steinbach, Plapp, Zhang. Acta Mat 2012;
Zhang, Steinbach. Acta Mat 2012

Redistribution within one reference volume (RV)

- No flux over the boundary
- Phase fractions are fixed inside the RV

P: inverse interface resistivity

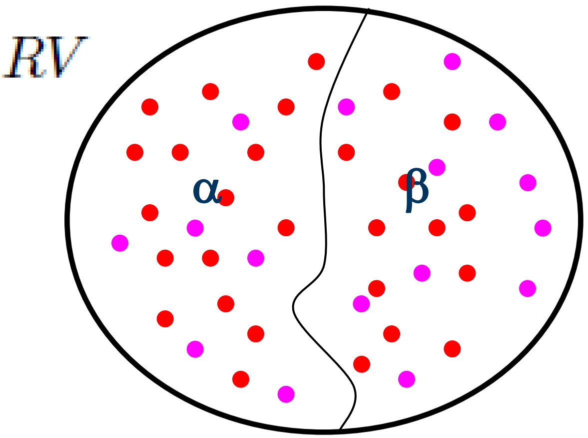


$$\phi_\alpha \dot{c}_\alpha = \underbrace{\vec{\nabla}\left(\phi_\alpha D_\alpha \vec{\nabla} c_\alpha\right)}_{=0} + P_{\alpha\beta}\phi_\alpha\phi_\beta\left(\tilde{\mu}_\beta - \tilde{\mu}_\alpha\right) + \underbrace{\phi_\alpha \dot{\phi}_\alpha (c_\alpha - c_\beta)}_{=0}$$

Redistribution within one reference volume (RV)

- No flux over the boundary
- Phase fractions can adjust with finite rate

P: inverse interface resistivity



$$\phi_\alpha \dot{c}_\alpha = \vec{\nabla}\left(\phi_\alpha D_\alpha \vec{\nabla} c_\alpha\right) + P_{\alpha\beta}\phi_\alpha\phi_\beta\left(\tilde{\mu}_\beta - \tilde{\mu}_\alpha\right) + \phi_\alpha\dot{\phi}_\alpha\left(c_\alpha - c_\beta\right)$$

$$\underset{0}{\shortparallel}$$

The relaxation model for c and Φ

The phase-field equation is modified according to the definition of driving force and phase-field mobility K

$$\dot{\phi}_\alpha = K\left\{\sigma_{\alpha\beta}\left[\nabla^2\phi_\alpha + \frac{\pi^2}{\eta^2}\left(\phi_\alpha - \frac{1}{2}\right)\right] + \frac{\pi^2}{8\eta}\left[f_\beta - f_\alpha - \left(\phi_\alpha\tilde{\mu}_\alpha + \phi_\beta\tilde{\mu}_\beta\right)\left(c_\beta - c_\alpha\right)\right]\right\}$$

$$\boxed{\Delta G_{\alpha\beta} = \Delta G_{\alpha\beta}^{\phi} + \Delta G_{\alpha\beta}^{Diff}}$$

$$\boxed{K = \frac{8P\eta\mu_{\alpha\beta}}{8P\eta + \pi^2\mu_{\alpha\beta}\left(c_\beta - c_\alpha\right)^2}}$$

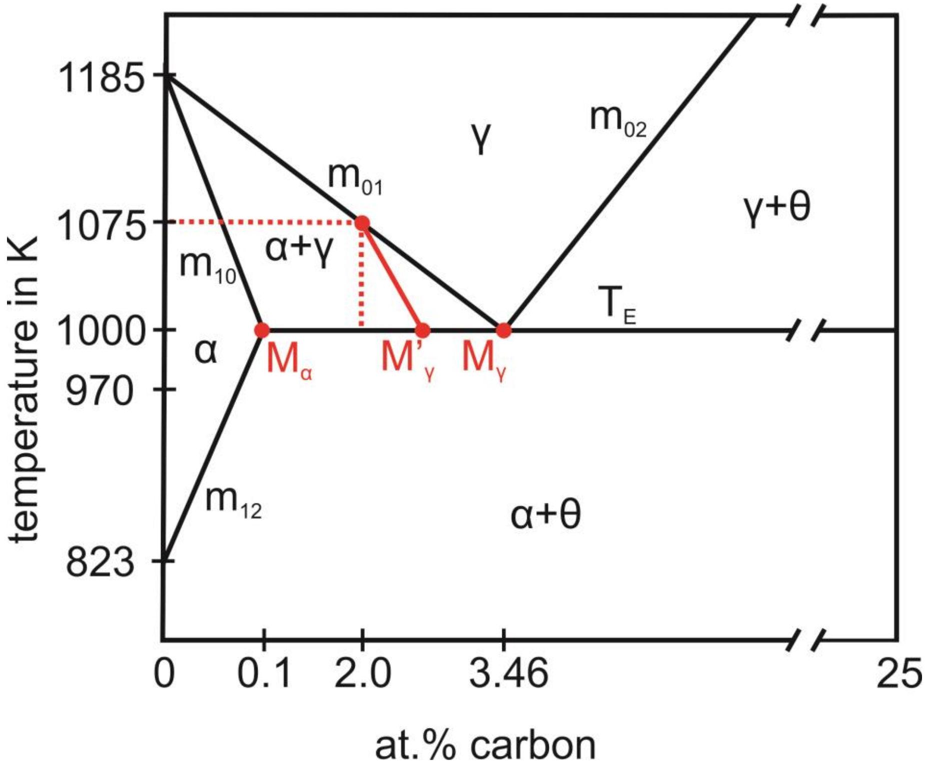
$P \to \infty$ The conventional model (two phases with same chemical potential) $K \to \mu_{\alpha\beta}$

$P \to 0$ Transformation can not proceed $K \to 0$

Ferrite growth simulation

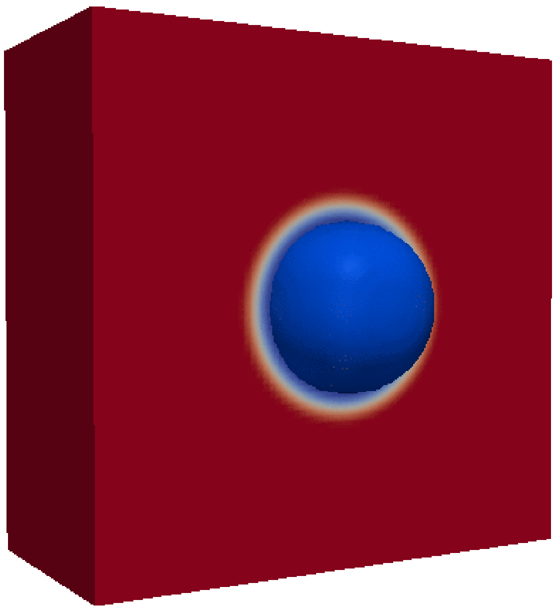
Example simulation:

- steel with 2 at-% C (hypoeutectoid)
- simulation starts at 1075 K in a box of austenite and one ferrite grain
- cooling with different cooling rates to eutectoid temperature

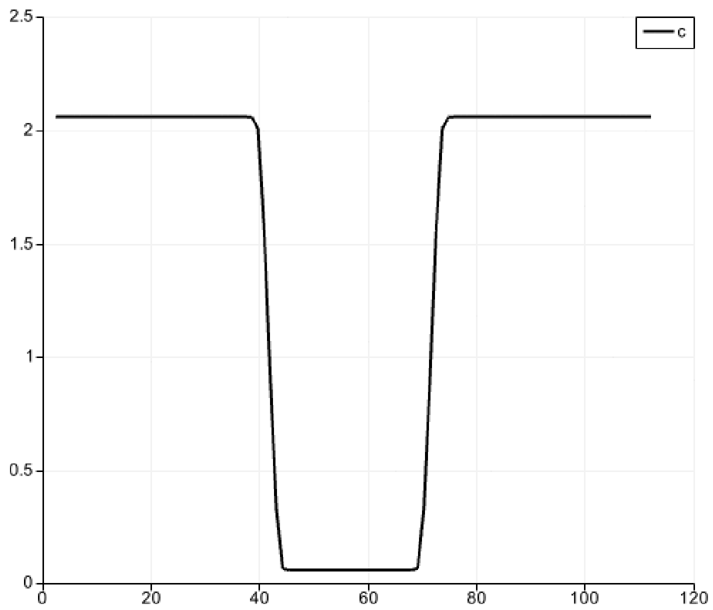


Ferrite growth simulation

Phase field



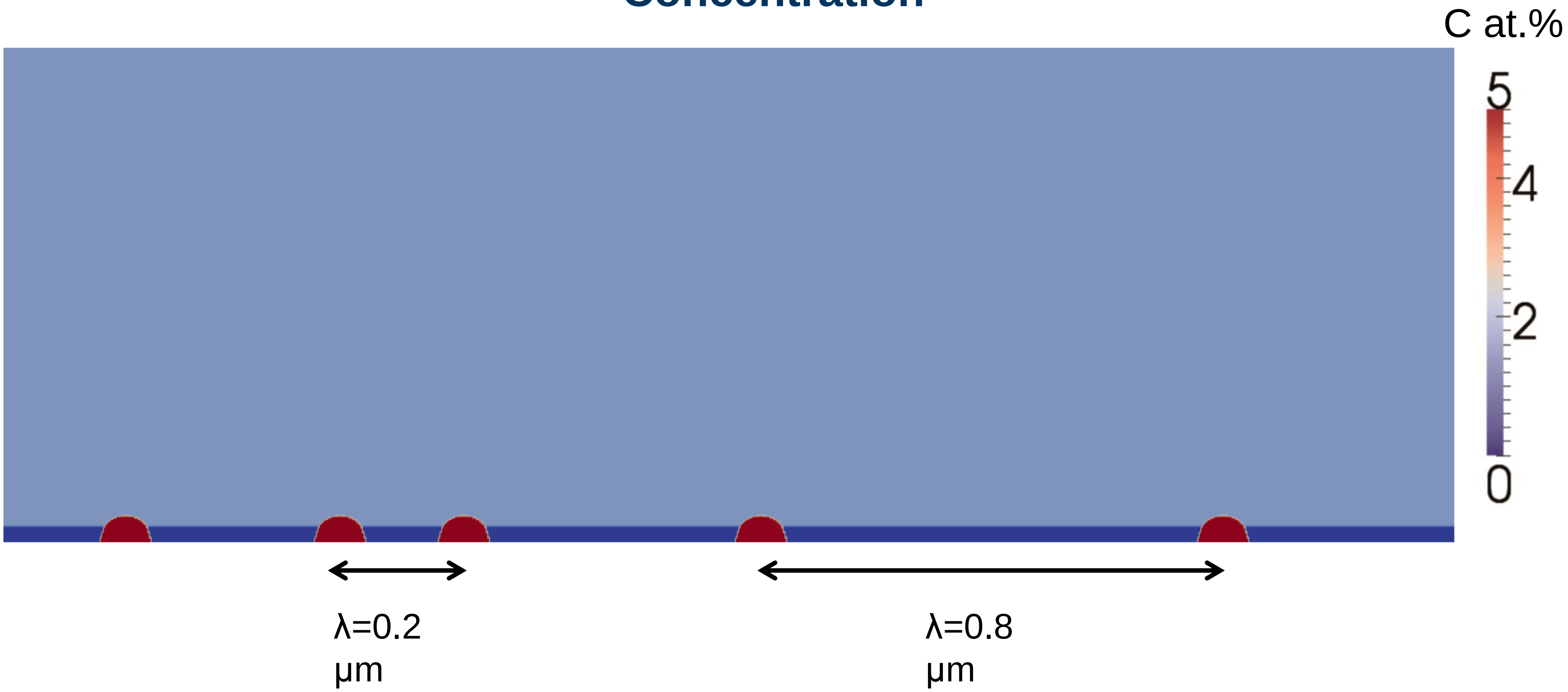
Carbon concentration [at.%]



R [K/s]	Equilibrium	0.5	1	5	10	50	100
C_γ [at-%]	3.46	3.42	3.39	3.32	3.05	2.32	2.15
$F_{pearlite}$ [%]	56.5	57.2	57.5	59.0	64.4	85.5	92.7

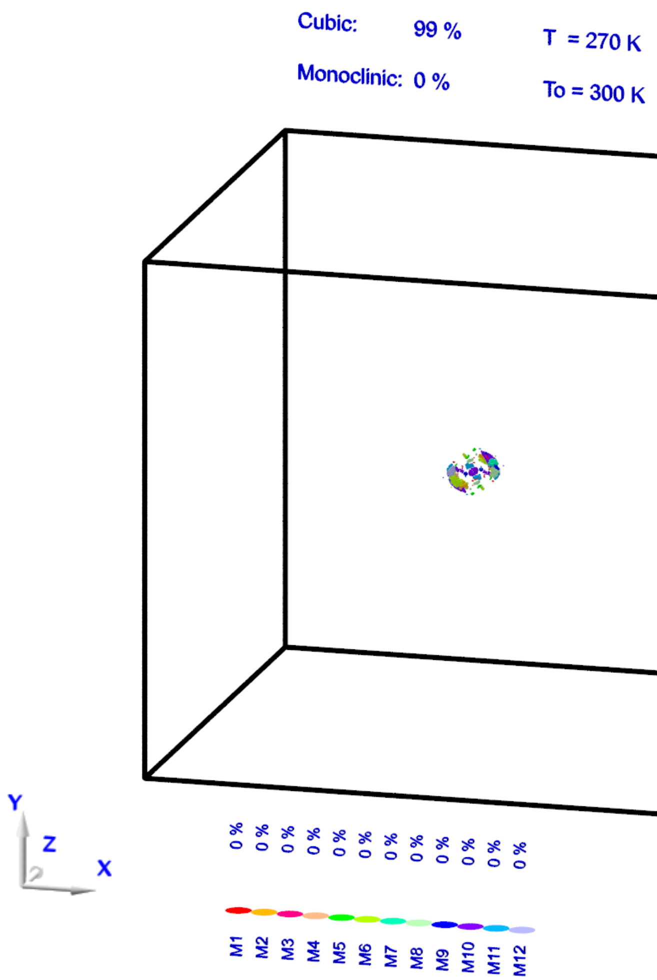
Pearlite growth simulation

Concentration



NiTi SMA

System size
512x**512**x**512**
grid points
(**1**x**1**x**1** µm)



Martensite Simulation (Steel)

?

Modeling transformations in steel

The necessary ingredients for successful modeling of solid-solid transformations in steel:

- **Phase field model for strongly non-equilibrium transformations**
- **Gibbs free energy dependence on local stress**

  It allows diffusion and transformations modeling under stress and in presence of defects

- **Incorporation of plastic relaxation mechanism**

  Is an absolute necessity for handling high strains associated with martensite and bainite formation or severe deformation during processing (recrystallization)

- **Investigation of the effect of dislocation density on equilibrium concentration of elements**

  Is a necessary ingredient for simulations of realistic concentration distributions in real structures

- **Tools and algorithms development**

  Any good model before being used should be implemented

Large deformations handling

Deformation decomposition:

homogeneous expansion

accumulated strain

$$f^{El} = \frac{1}{2}\underbrace{\left[\varepsilon_i^{tot} - \left(\varepsilon_i^{*} - \bar{\varepsilon}_i - \varepsilon_i^{rot} + \varepsilon_i^{acc}\right)\right]}_{\varepsilon_i^{elast}} C_{ij}\left[\varepsilon_j^{tot} - \left(\varepsilon_j^{*} - \bar{\varepsilon}_j - \varepsilon_j^{rot} + \varepsilon_i^{acc}\right)\right]$$

eigenstrain

rotation

Local deformation accumulation:

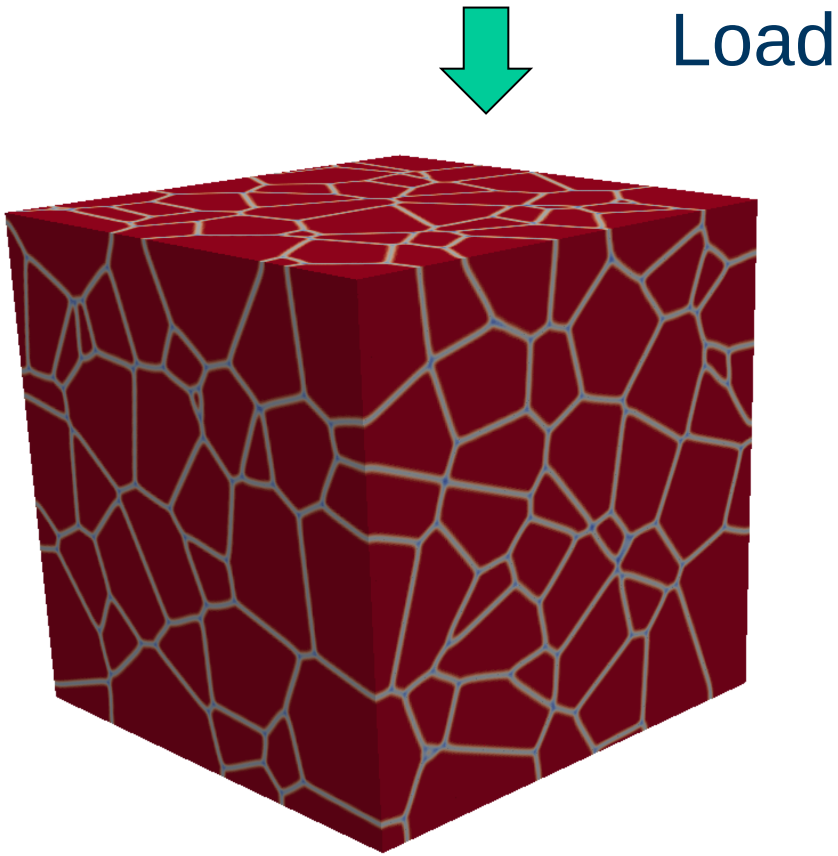
strain accumulated in one time step

$$\bar{\varepsilon}_{new}^{acc} = \bar{\varepsilon}_{old}^{acc} + ln\left(1 + \Delta\varepsilon^{acc}\right)$$

Explicit rotation of sensitive tensors and properties:

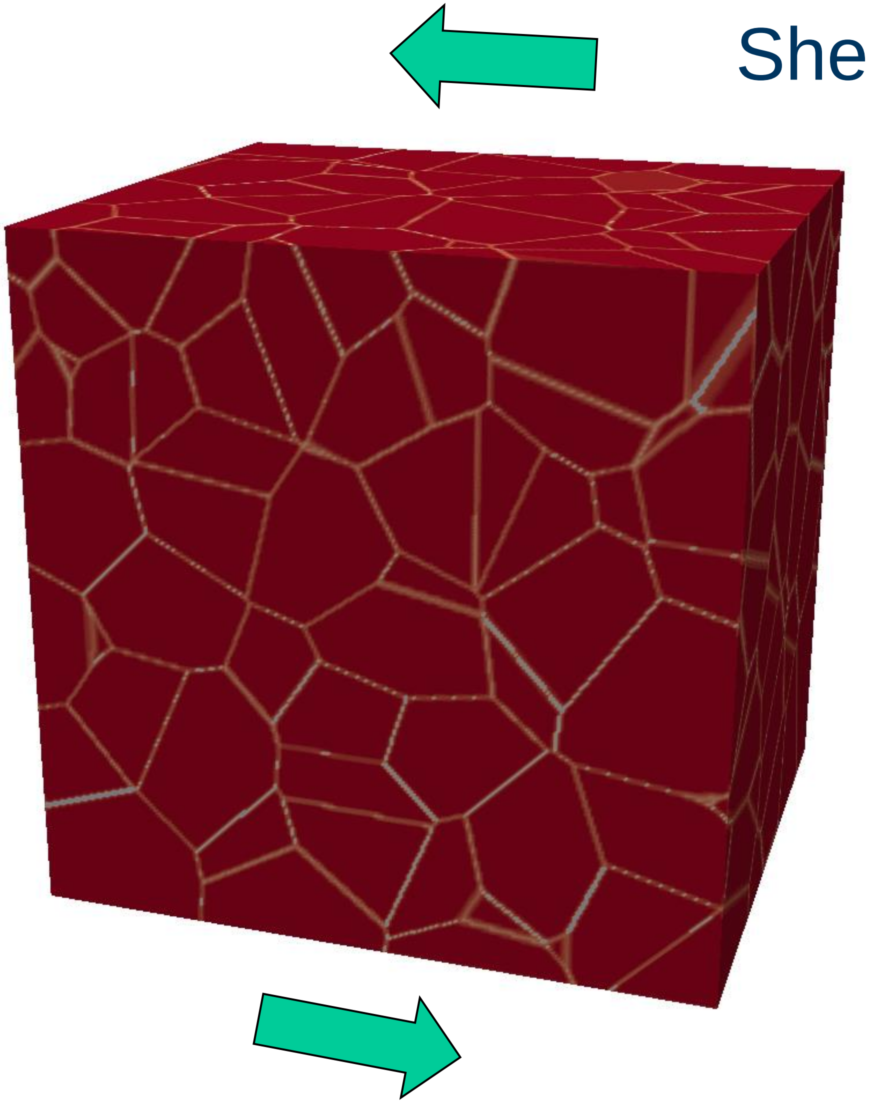
C_{ij}, ε_i^{*}, ε_i^{acc}, ε_i^{plast}, slip systems, anisotropic interface properties, etc.

"Hot roling"



"Slip"

Shear



Summary

- New phase field model suitable for simulations of highly non-equilibrium transformations is presented.
- The main features of the model are yet to be explored but it already shows great potential for simulations of transformations in steel
- In order to model steel transformation incorporation of elastic and plastic effects on diffusion, and evolution of phase and grain boundaries in one simulation is required
- There is a need for new algorithms and new models in order to improve current modeling techniques

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www.OpenPhase.de

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Thank you for your attention!