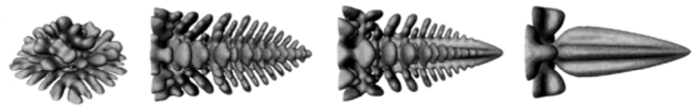
Phase-field simulation of solid state transformation with thermo-mechanical interaction

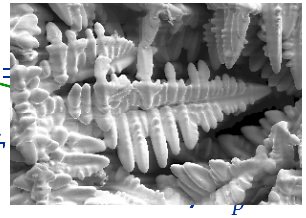
Ingo Steinbach

ICAMS
INTERDISCIPLINARY CENTRE FOR ADVANCED MATERIALS SIMULATION

RUHR UNIVERSITÄT BOCHUM RUB

Thermal dendrites: Ryo Kobayashi 1994

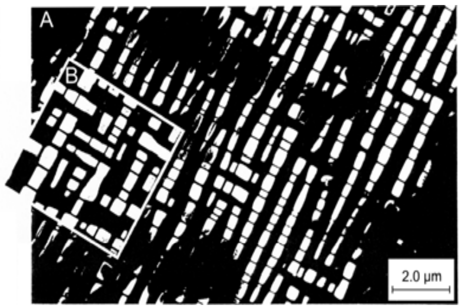




$\tau\dot{\phi} =$

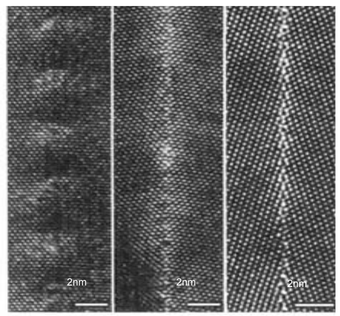
$\dot{T}$

γ' precipitates in Ni-base superalloys:
Y. Wang, L.Q. Chen, A.G. Khachaturyan 1995



Ni-base super alloy: alligned cuboids in crystallograpic directions

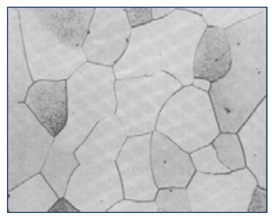
Grain boundary structure



5.0° 20.0° 39.0° Σ9

TEM Picture
<110> tilt grain boundary
in ZrO_2

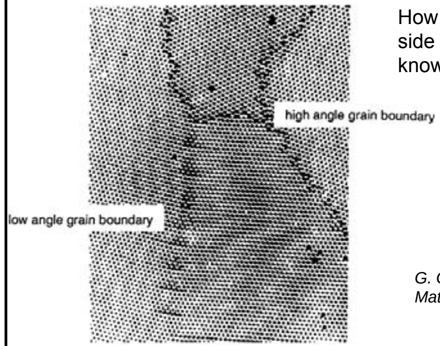
Y. Ikuhara, N. Shibata, T. Watanabe, F. Oba, T. Yamamoto and T. Sakuma, Ann. Chim. Sci. Mat., 2002,27 Suppl 1:S21-30



Grain boundaries in ferrite

Curvature driven flow

Phenomenological picture $V = \mu\sigma \cdot \kappa$

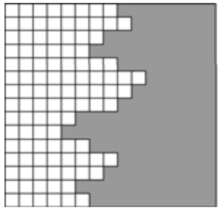


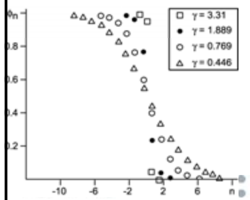
How does an atom close on one side of a grain boundary know its mean curvature?

G. Gottstein, Physical Foundation of Materials Science, Springer

Curvature driven flow

Mechanistic picture: The atoms at grain boundaries jump between lattice sites of the adjacent crystals





Characteristic function Φ indicates the belonging of one atom to one crystal respectively

$$\dot{\phi} \propto \nabla^2 \phi$$

The belonging to one crystal is favourable

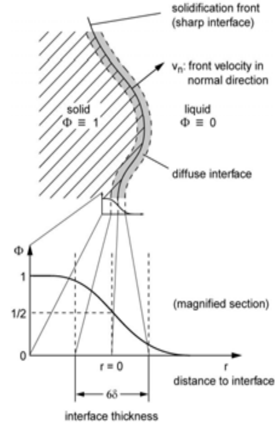
$$\dot{\phi} \propto \phi(1-\phi)(0.5-\phi)$$

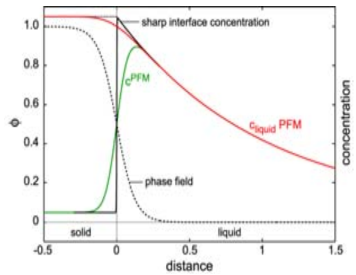
The balance between both actions leads to a stable interface

Outline

- Basics of "phase-field" models
- Elastic interactions
- Examples:
    - Pearlite
    - Strain stabilized precipitation

Diffuse interface with steep concentration profile

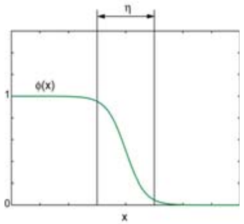




Concentration profile through the interface

Phase-field model in the Gibbs-Thomson limit

„Order parameter“ Φ, the „Phase-Field“ variable



$$F=\int_\Omega d^3x\,\frac{\varepsilon}{2}\left|\nabla\phi\right|^2+\gamma\phi^2(1-\phi)^2\;+m\,\phi\;+f_0$$

$$F=\int_\Omega d^3x\,\frac{\sigma}{\eta}\left[\left|\nabla\phi\right|^2\eta^2+72\phi^2(1-\phi)^2\right]+\phi\,\Delta G_{\alpha\beta}(c_\alpha,c_\beta)+G_0+\tilde{\mu}\left(c-\phi c_\alpha-(1-\phi)c_\beta\right)$$

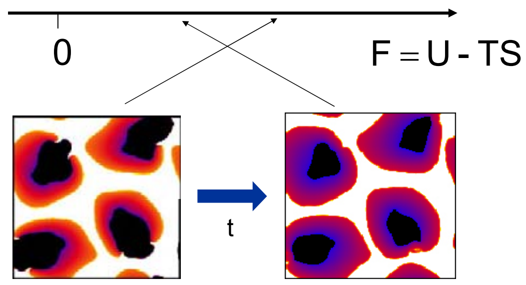
$$v=\dot{\phi}\Big/\left|\nabla\phi\right|=\mu\left(\kappa\,\sigma+\Delta G_{\alpha\beta}\right)$$

σ: interface energy
μ: interface mobility
η: interface thickness
$\Delta G_{\alpha\beta}$: Gibbs energy difference
$\tilde{\mu}$: diffusion potential

Caginalp et Fife 1986, Wheeler et al. 1992

The phase-field functional

"A functional is a unequivocal mapping of a space of functions ϕ(x) on to real numbers"

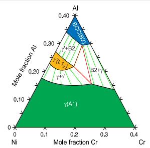


Background of “phase-field”: The common model philosophy

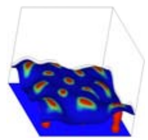
Thermodynamic principle	$\tau\dot{\phi}=-\frac{\delta F}{\delta\phi}$
Material specific Model of the Free energy functional	$F=\int_V dv\,\tilde{f}(\phi,c,T\ldots)$
Mathematical rigorous derivation of the "thin interface limit"	$\dot{\phi}=\mu(\sigma\kappa+\Delta G)\left|\nabla\phi\right|$
Numerical sound solution	$\kappa_i=\frac{\sum_i \phi_j-\phi_i}{\phi_i(1-\phi_i)\cdot\Delta x^2}-\frac{(1-2\phi_i)}{\eta^2}\cdot 8$

μ: interface mobility;
η: interface thickness
ΔG: thermodynamic undercooling;
σ: interface energy;
κ: interface curvature;
Δx: numerical discretization

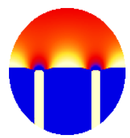
Multi-phase-field model coupled to solute diffusion



$$F=\int d\Omega\left(\sum_{\alpha,\beta}\frac{\sigma_{\alpha\beta}(\vec{n}_\alpha,\vec{n}_\beta)}{\eta_{\alpha\beta}}K_{\alpha\beta}(\nabla\phi_\alpha,\nabla\phi_\beta,\phi_\alpha,\phi_\beta)+\sum_\alpha\phi_\alpha f_\alpha\left(\vec{c}_\alpha\right)\right)$$



$$\dot{\phi}_\alpha=\frac{-1}{n}\sum_\beta\mu_{\alpha\beta}\left(\frac{\delta F}{\delta\phi_\alpha}-\frac{\delta F}{\delta\phi_\beta}\right)$$



$$\dot{c}^i=\sum_{k=1}^{m}\nabla M^{ik}\,\nabla\frac{\delta F}{\delta c^k}=\sum_{k=1}^{m}\sum_{\alpha=1}^{n}\nabla\phi_\alpha\,D_\alpha^{ik}\,\nabla c_\alpha^k$$

Steinbach MSMSE 2009

Free boundary problem of crystallization: the „Stephan problem“

temperatur

1)2) $\rho c_p \dot{T} = \lambda \Delta T + L_0 \dot{\phi}$

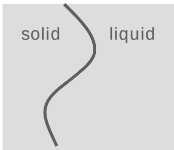
energy ballance

2) $L_0 \cdot v = \lambda_{liq} \cdot \nabla T|_{liq} - \lambda_{sol} \cdot \nabla T|_{sol}$

Gibbs-Thomson equation

3) $v = \mu(-\Gamma\kappa + T_{eq} - T_{intf})$

3‘) $\dot{\phi} = \mu\left\{\Gamma\left(\Delta^2\phi - \frac{\pi^2}{2\eta^2}\left(\frac{1}{2} - \phi\right)\right) + \Delta\phi(T_{eq} - T_{intf})\right\}$



v : velocity of the interface
κ : curvature

λ: heat conductivity
ρc_p: specific heat
L_0: latent heat
Γ: Gibbs-Thomson coeffizient

Outline

- Basics of “phase-field” models
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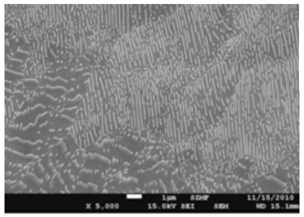
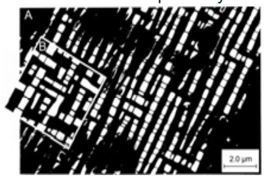
- Examples:
  - Pearlite
  - Strain stabilized precipitation

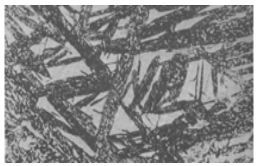
Motivation I: Phase distribution in solid state

Pearlite, courtesy Benteler

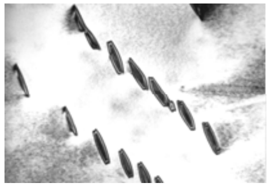


Ni-base super alloy



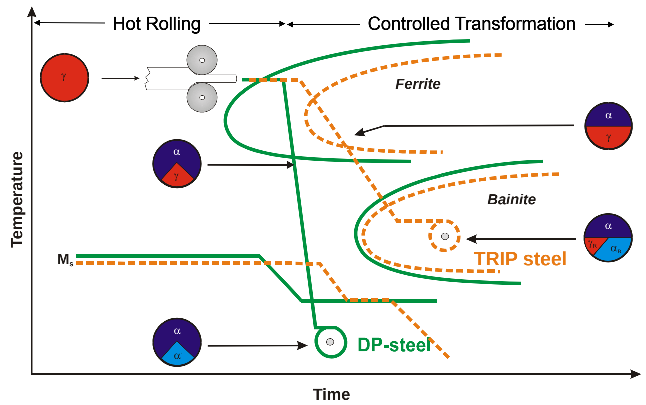


Bainite



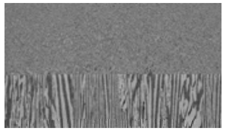
NiTi precipitates, courtesy Eggeler

Motivation II: Processing of multiphase steels



Mechanisms of Microstructure Formation

microstructure formation



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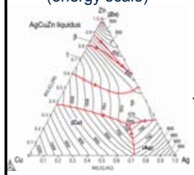
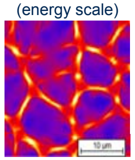
thermodynamics (energy scale)



+

mechanical equilibrium (energy scale)



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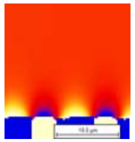
transport / diffusion (time scale)



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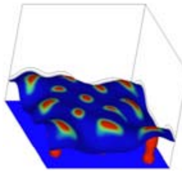
interfaces (length scale)



TQ interface from TCS | stress/strain solver | diffusion solver | phase field method

OpenPhase

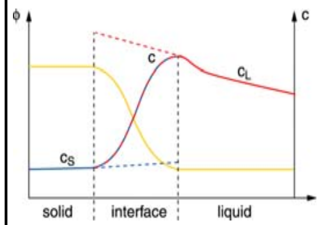
Homogenization of stress/strain in the interface region

$$f^{el} = \sum_\alpha \phi_\alpha \frac{1}{2}\left(\varepsilon_\alpha - \varepsilon_\alpha^*\right) C_\alpha \left(\varepsilon_\alpha - \varepsilon_\alpha^*\right)$$

discontinuity of strain $\varepsilon_\alpha \neq \varepsilon_\beta$

or

discontinuity of stress $\sigma_\alpha \neq \sigma_\beta$



WBM 1994:	$c_L = c_S = c$
Multi-phase-field:	$c = \phi_L \cdot c_L + \phi_S \cdot c_S$
Tiaden 1969	$c_L = k c_S$
Kim 1999	$\mu_L(c_L) = \mu_S(c_S)$

Reuss limit of continuous stress

$$f^{el} = \sum_\alpha \phi_\alpha \frac{1}{2}\left(\varepsilon_\alpha - \varepsilon_\alpha^*\right) C_\alpha \left(\varepsilon_\alpha - \varepsilon_\alpha^*\right)$$

discontinuity of strain $\varepsilon_\alpha \neq \varepsilon_\beta$

! continuity of stress between the phases

$$\sigma \overset{!}{=} \sigma_\alpha = \frac{\delta f^{el}}{\delta \varepsilon_\alpha} \longrightarrow f^{el} = \frac{1}{2}\left(\varepsilon - \varepsilon^*\right)\hat{C}\left(\varepsilon - \varepsilon^*\right)$$

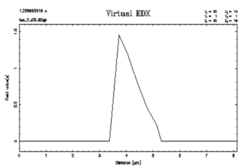
$$\hat{C} = \left[\sum_\alpha \frac{\phi_\alpha}{C_\alpha}\right]^{-1}; \qquad \varepsilon^* = \phi_\alpha \varepsilon_\alpha^*; \qquad \varepsilon_\alpha = \frac{\hat{C}}{C_\alpha}\left(\varepsilon - \varepsilon^*\right) + \varepsilon_\alpha^*$$

Hooks matrix is a homogenous mixture between phases

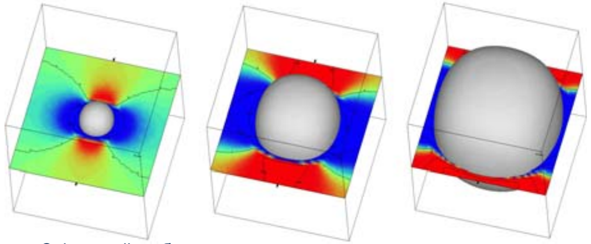
Reuss limit of continuous stress

$$f^{el} = \frac{1}{2}\left(\varepsilon - \varepsilon^*\right)\hat{C}\left(\varepsilon - \varepsilon^*\right)$$

$$\left(\frac{\partial}{\partial \phi_\alpha} - \frac{\partial}{\partial \phi_\beta}\right) f^{el} = \Delta G_{\alpha\beta}^{el} = \left(\varepsilon - \varepsilon^*\right)\hat{C}\left[\left(\varepsilon_\alpha^* - \varepsilon_\beta^*\right) - \frac{1}{2}\left(\frac{1}{C_\alpha} - \frac{1}{C_\beta}\right)\hat{C}\left(\varepsilon - \varepsilon^*\right)\right]$$



Verification: growth of a single particle in a matrix

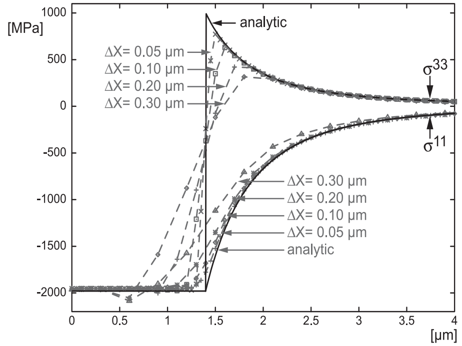


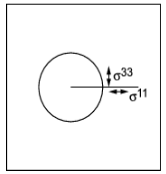
Colour coding: σ_{yy}

Elasticity moduli: C_{11} = 280GPa, C_{12} = 120GPa, Eigenstrain = 1%

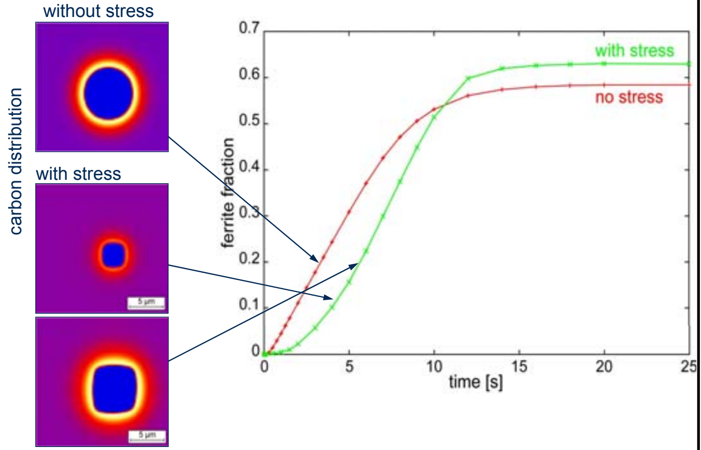
Thermodynamic data of Fe-$C_{0.463at\%}$-$Mn_{0.496at\%}$, TCFe3 database

Test against analytical solution (Eshelby)

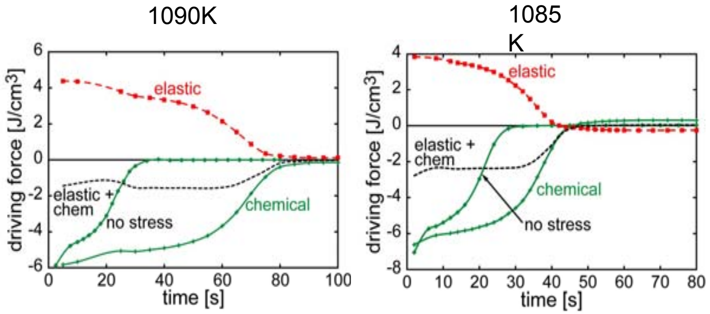




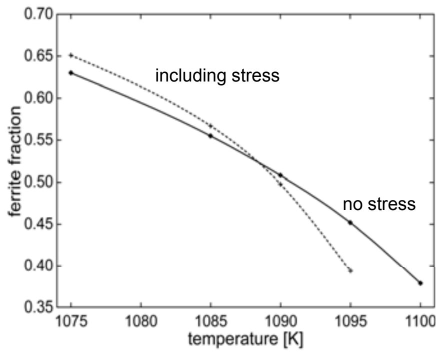
Isothermal transformation: Growth of a single ferrite precipitate



Evolution of the driving forces during transformation



Dependence of equilibrium fraction on internal stress



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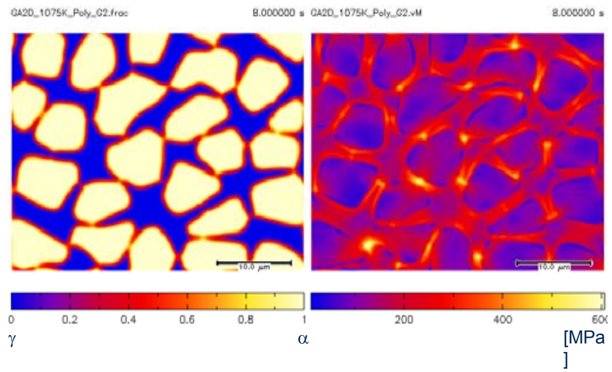
γ/α Transformation



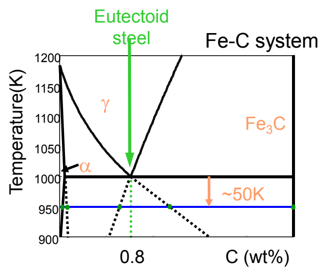
ICAMS 26 RUB

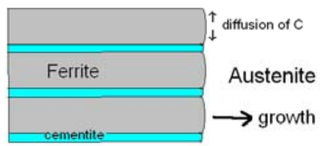
Outline

- Basics of "phase-field" models
- Elastic interactions
- Examples:
  - Pearlite
  - Strain stabilized precipitation

ICAMS 27 RUB

Pearlite





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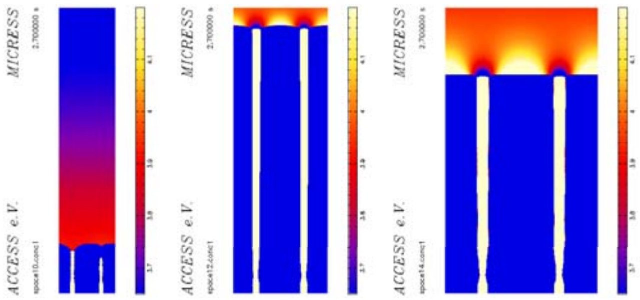
Pearlite

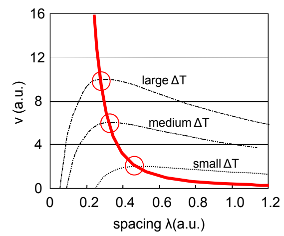


Phase-field calculation of diffusion controlled growth of pearlite with different spacings *(Nakajima et al. 2006)*

Pearlite

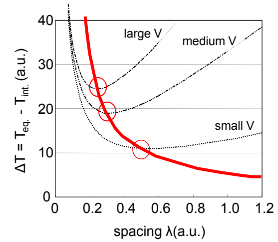
The "Zener-Hillert-Tiller-Jackson-Hunt“ Model
1946 1957 1958 1966

Pearlitic: ΔT= const.



$a_1 v = \Delta T/\lambda - a_2/\lambda^2$

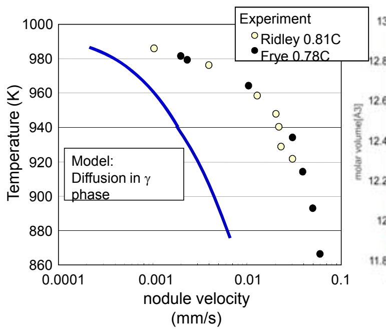
Eutectic: v= const.

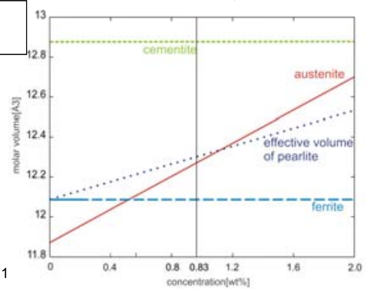


$\Delta T = a_1 v \lambda + a_2/\lambda$

Transformation strain and concentration dependent strain

Lattice constants:		
	austenite	a = 2.301 Å/atom
	ferrite	a = 2.298 Å/atom
	cementite	a = 1.98 Å/atom; b = 2.23 Å/atom; c = 2.953 Å/atom





Phase-field model coupled to elastic strain

$$f = f^{i} + f^{ch} + f^{el}$$

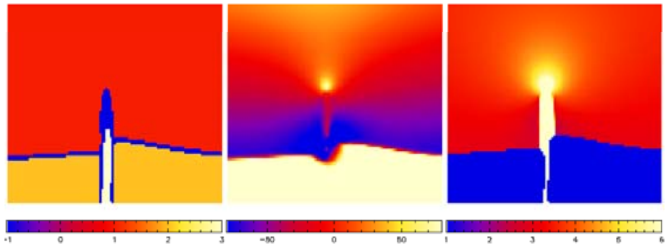
$$f^{el}(x,t) = \sum_{\alpha} \phi_\alpha(x,t)\frac{1}{2}\left(\varepsilon_\alpha(x,t) - \varepsilon_\alpha^{*} - \varepsilon_\alpha^{1} c_\alpha(x,t)\right) C_\alpha \left(\varepsilon_\alpha(..) - \varepsilon_\alpha^{*} - \varepsilon_\alpha^{1} c_\alpha(..)\right)$$

$$\dot{\phi}_\alpha = \frac{1}{n}\sum_{\beta} \mu_{\alpha\beta}\left(\frac{\delta f}{\delta\phi_\alpha} - \frac{\delta f}{\delta\phi_\beta}\right) = \frac{1}{n}\sum_{\beta}\mu_{\alpha\beta}\left(I_{\alpha\beta} + \Delta G_{\alpha\beta}^{chem} + \Delta G_{\alpha\beta}^{el}\right)$$

$$\dot{c} = \sum_{\alpha} \nabla M\, \phi_\alpha \nabla \frac{\delta f}{\delta c_\alpha} = \sum_{k=1}^{m} \nabla M\, \phi_\alpha \left(\frac{\delta^2 f}{\delta c_\alpha^2}\nabla c_\alpha + \varepsilon_\alpha^{1} \nabla\sigma\right)$$

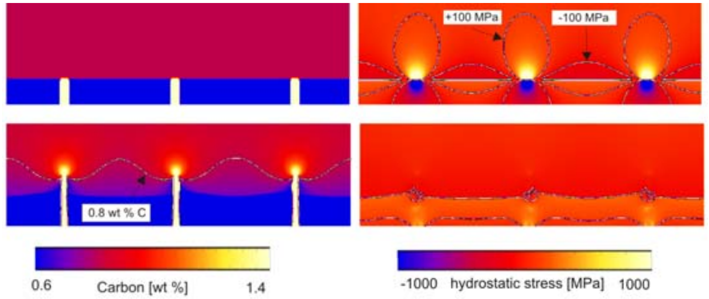
$$0 = \nabla\frac{\partial f}{\partial \varepsilon} = \nabla\sigma = \sum_{\alpha} \nabla\phi_\alpha C_\alpha \left(\varepsilon_\alpha - \varepsilon_\alpha^{*} - \varepsilon_\alpha^{1} c_\alpha\right)$$

The effect of transformation strain on growth

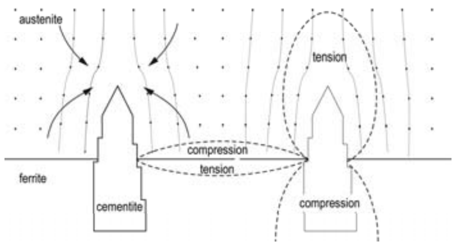


Phase distribution Hydrostatic stress Carbon concentration

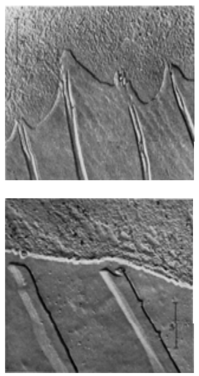
The effect of transformation strain on growth



The effect of transformation strain on growth

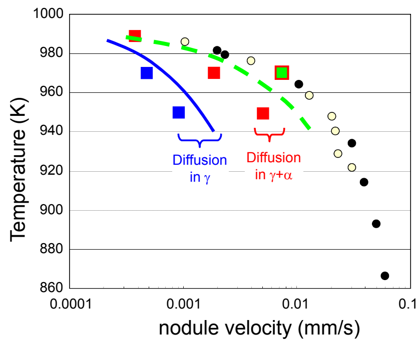


staggered growth mechanism of pearlite



quenched pearlite front
(Darken,Fisher 1960)

The effect of transformation strain on growth

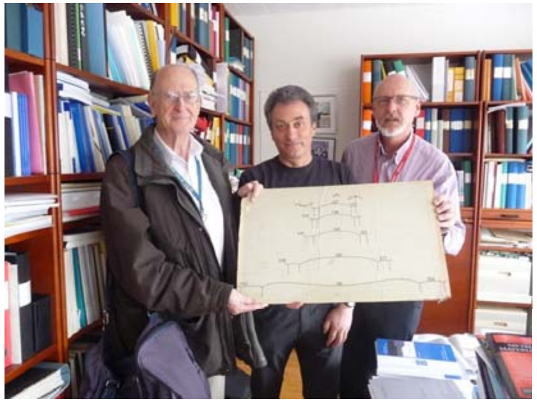


Experiment
- ○ Ridley 0.81C
- • Frye 0.78C

Phase Field Calculation
- ■ Diffusion in γ phase
- ■ Diffusion in γ and α phase
- – – + Diffusion due to Stress (extrapolated)
- ■ + transformation strain
- + faceted anisotropy of cementite

Model
- — Diffusion in γ phase

Mats Hillert IS John Ågren

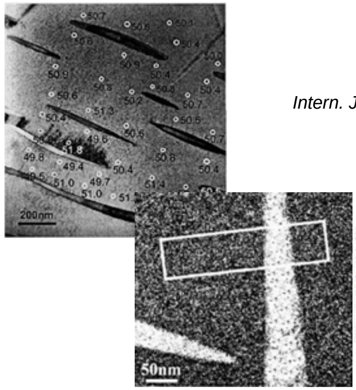


Stokholm 2009

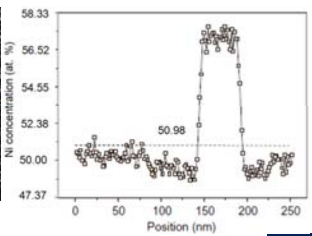
Outline

- Basics of "phase-field" models
- Elastic interactions
- Examples:
  - Pearlite
  - Strain stabilized precipitation

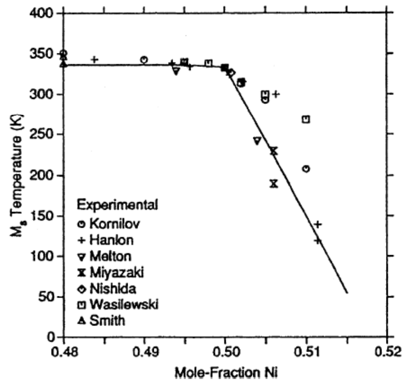
Precipitation in Ni-Ti shape memory alloys: experimental observations



Experiment:
Yang, Schryvers,
Intern. Journ. Of Appl. Electromagn. And Mech. 23 (2006) p. 17

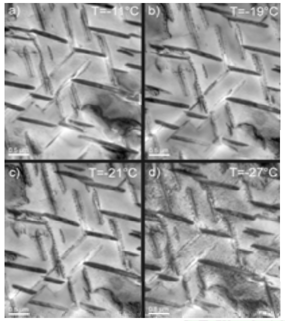


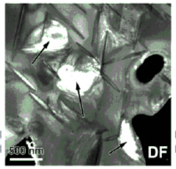
Martensite Start Temperature

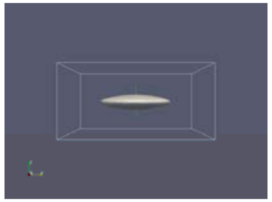


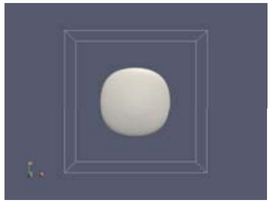
Otsuka, Ren
Progress in Material Science 50 (2005), p. 511

Ni4-Ti3 precipitate in NiTi

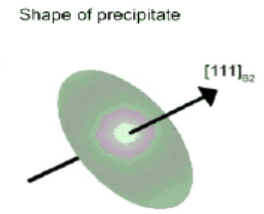


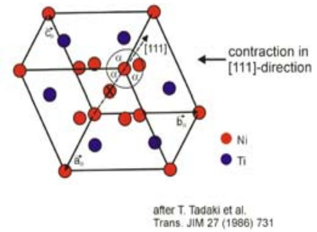






Ni4-Ti3 precipitate in NiTi



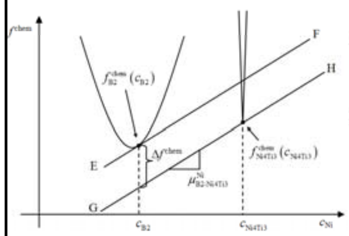


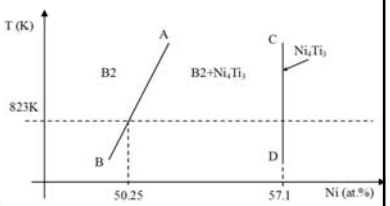
Initial conditions

- Ni_4Ti_3 precipitates in the Ni oversaturated B2 matrix
  - $C_{B2,0}$ = 51.0 at.%
  - $C_{Ni_4Ti_3}$ = 57.1 at.%
- Diffusion controlled precipitate growth
  - Diffusion only in the matrix, no diffusion in the stoichiometric phase
- Lattice mismatch
  - Anisotropic eigenstrains:

$$\epsilon^*_{Ni_4Ti_3} = \begin{bmatrix} -0.00438 & 0 & 0 \\ 0 & -0.00438 & 0 \\ 0 & 0 & -0.02688 \end{bmatrix}$$

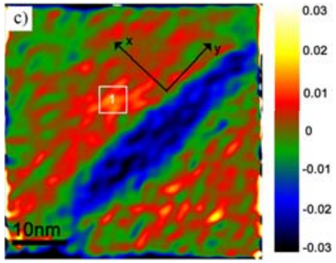
The phase diagram





Results: Strain in the matrix

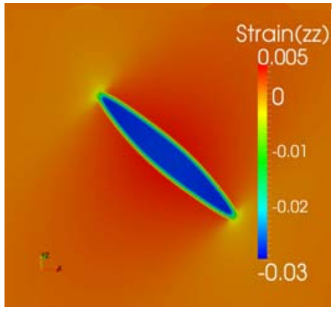
Simulation: Guo et al., Acta Mater. 59 (2011) p. 3287



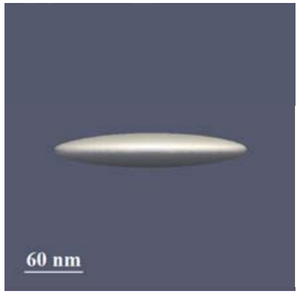
Strain (zz)

Experiment: Tirry, Schryvers; Nature Mater 8 (2009) 752

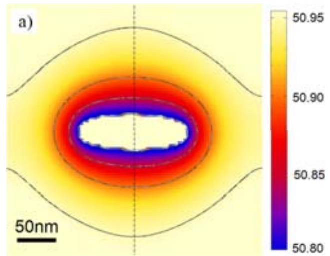
Simulation: Strain (zz)



Results concentration in the mattrix



Phase field



Ni Concentration

Concentration Dependent Elastic Coefficients

Larche , Cahn 1982: The effect of self-stress on diffusion in solids

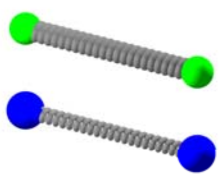
$$\dot{c}^i = \nabla M^{ik} \nabla \frac{\delta f}{\delta c^i} = \nabla M^{ik} \nabla \left(\frac{\delta f^{chem}}{\delta c^i} + \frac{\delta f^{mech}}{\delta c^i} \right)$$

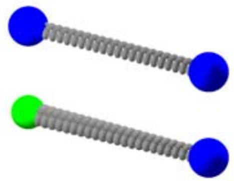
$$= \nabla M^{ik} \left(\frac{\delta^2 f^{chem}}{\delta c^{i^2}} \nabla c + \kappa \nabla f^{mech} \right)$$

Elastic coefficients: Pure elements and the alloy

$C^{ijkl}_{Ti} < C^{ijkl}_{Ni}$

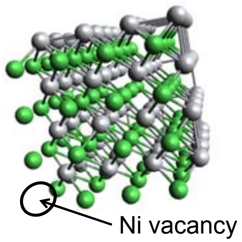
$C^{ijkl}_{NiTi} = C^{ijkl}_{NiTi}(c_{Ni})$





Elastic Properties of B2 Ni-Ti with Defects

- Perform full relaxation of B2 NiTi supercells with vacancies and substitutions to compare changes in elastic energy
- Obtain DFT elastic properties as a function of Ni-concentration
- Use DFT elastic properties and trends as inputs for phase-field (PF) models



1) Obtain DFT C_{ij} as function of Ni-concentration
2) Import concentration dependent C_{ij} into PF-model
3) Incorporate into PF mechanical energy term

$$E(V,\alpha) = E(V_o,0) + V_o\left(\sum_i \tau_i\alpha_i + \frac{1}{2}\sum_{i,j} C_{ij}\alpha_i\xi_i\alpha_j\xi_j\right)$$

$$C^{ijkl} = \sum_{\alpha=1}^{N} \phi_\alpha C_\alpha^{ijkl} = \sum_{\alpha=1}^{N} \phi_\alpha C_{\alpha,0}^{ijkl}[1 + \kappa_q^\alpha \Delta c^\alpha]$$

$$f^{mech} = \frac{1}{2}\sum_{\alpha=1}^{N} \phi_\alpha [\epsilon_\alpha^{ij} - \epsilon_\alpha^{*ij}]\, C_\alpha^{ijkl}(\bar{c}_\alpha)\, [\epsilon_\alpha^{kl} - \epsilon_\alpha^{*kl}]$$

Concentration Dependent Elastic Coefficients

- Linear coupling between the elastic coefficients and the Ni concentration:

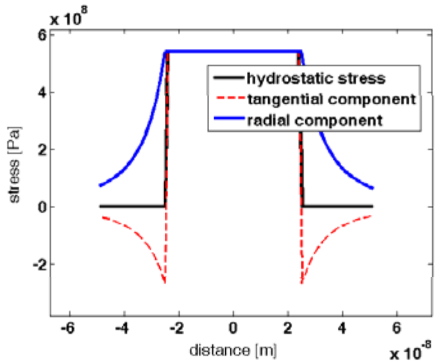
$$C^{ijkl}(c) = \sum_{\alpha=1}^{N} \phi_\alpha C_\alpha^{ijkl}(c) = \sum_{\alpha=1}^{N} \phi_\alpha C_{\alpha,0}^{ijkl}(1 + K^\alpha \Delta c^\alpha)$$

- Elastic contribution to the fluxes:

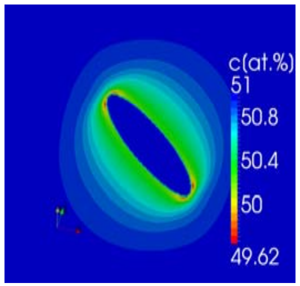
$$j = \nabla\left[M\frac{\partial f^{CH}}{\partial c} + M\frac{\partial f^{EL}}{\partial c}\right]$$

$$= j_{Diff} + M\underbrace{\frac{\partial \epsilon^{ij}}{\partial c}}_{=0}\nabla\sigma^{ij} + MK\nabla\left[\epsilon^{ij}C_0^{ijkl}\epsilon^{kl}\right] - c_\alpha^0$$

The role of hydrostatic stress

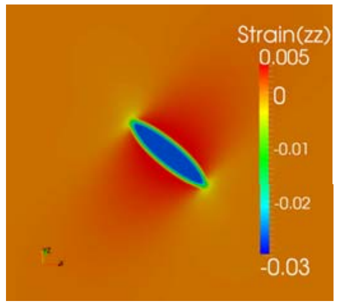


Simulations with concentration dependent elasticity (K=2e-3)

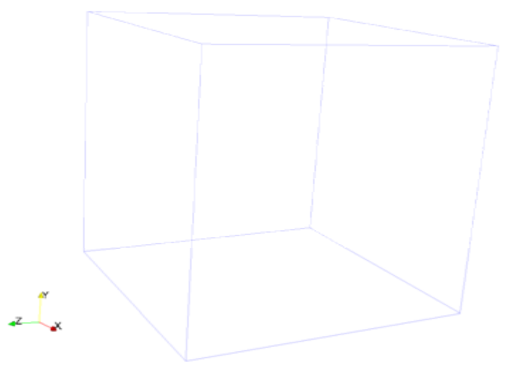


Ni Concentration

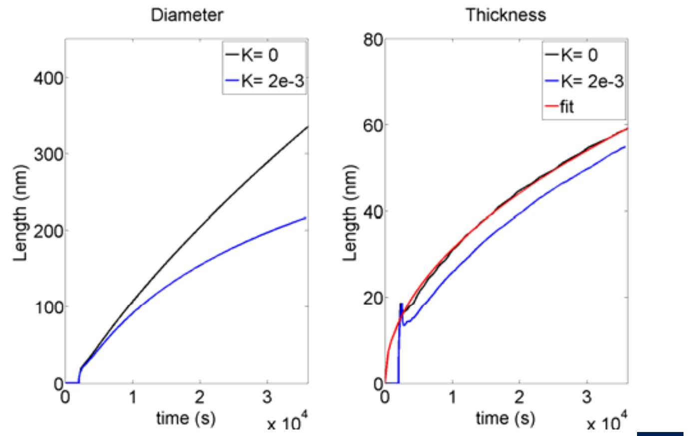
Strain (zz)



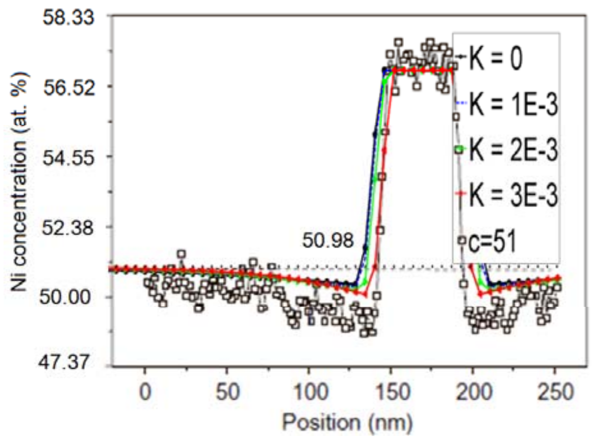
Growth kinetics



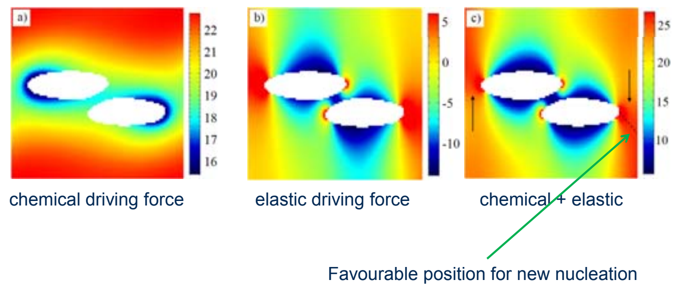
Growth kinetics



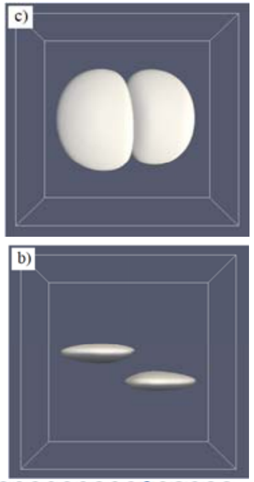
Concentration profile



Autocatalytic nucleation: driving force for nucleation



Autocatalytic nucleation



Experiments Eggeler, Bochum

Conclusion

- Solid state transformations cannot be well understood without the consideration of stress-strain effects.
- The phase-field method provides a thermodynamic consistent framework for the investigation of phase transformations subject to elastic effects.
- Examples were presented which demonstrate the predictive capability of the approach.

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Precipitation of γ' in a Ni-Al alloy