FROM FIRST PRINCIPLES TO MULTI-SCALE MODELING OF MATERIALS,
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Phase-Field Modeling of Technical Important Alloys

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access

Outline

1. Introduction
2. Pragmatic Multi-Phase-Field Model
3. Coupling to Thermodynamic Data: Quasi-Equilibrium
4. Simulation of Technical Alloys and Processes: Examples
    a) Linking to the Process: The General Micro-Macro Problem
    b) ”Bridgman” Approximation: Directional Solidification
    c) “DTA” Approximation: Small Samples
    d) Homoenthalpic Approximation: External 1D-Temperature Field
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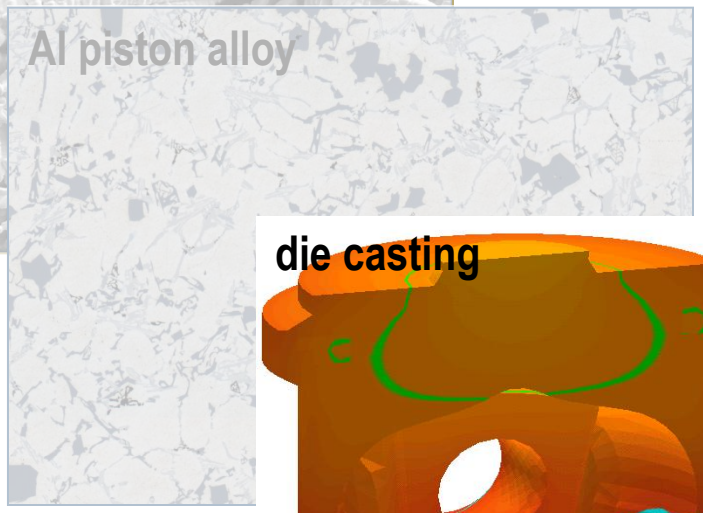
Introduction: Phase-Field Simulation of Complex Technical Microstructures

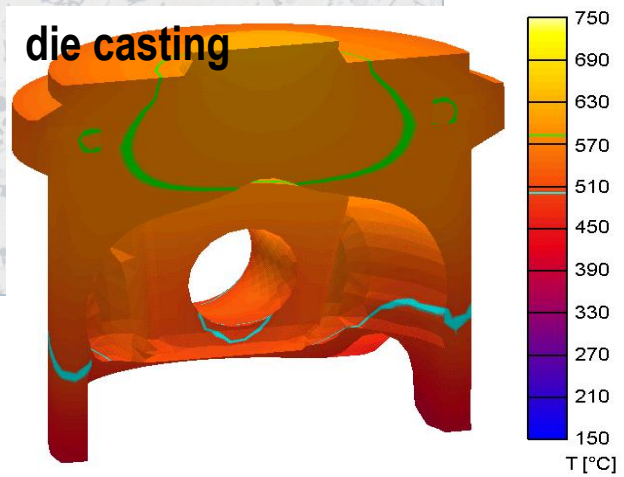
Challenges linked with simulation of technical microstructures:

- complex alloys
  - complex morphologies
    - complex thermodynamics
      - complex processes

carbon steel

Fe	C	Si	Mn	P	S	Al	Cr	Cu	Mo	N	Ti	Ni
Bal.	0,225										0038	0,021





→ ‘pragmatic’ phase-field approach

Introduction: Pragmatic Phase-Field Approach

What is a ‘pragmatic’ phase-field approach?

- multiphase-field model which allows simulation on µm scale
- online-coupling to off-the-shelf thermodynamic and diffusion databases
- advanced thermal coupling to external process conditions
- pragmatic simulation strategy (calibration, simplifications)
- robust multi-purpose code (no dedicated solutions)

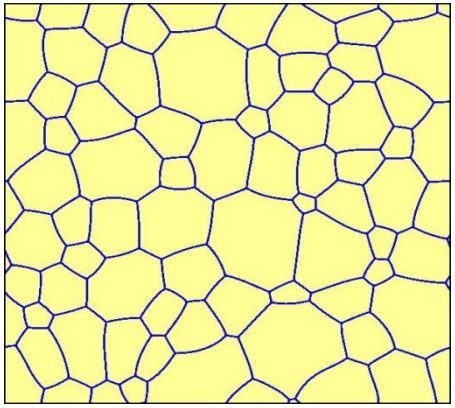
→ **MICRESS®**

The Software MICRESS®

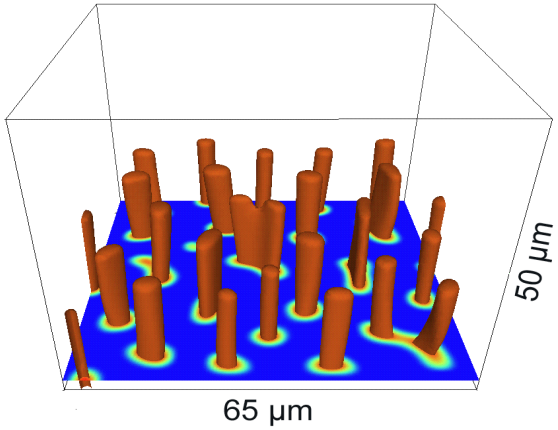
MICRESS: MICRostructure Evolution Simulation Software

Can be applied to composition, temperature or curvature controlled transformations on the microscale:

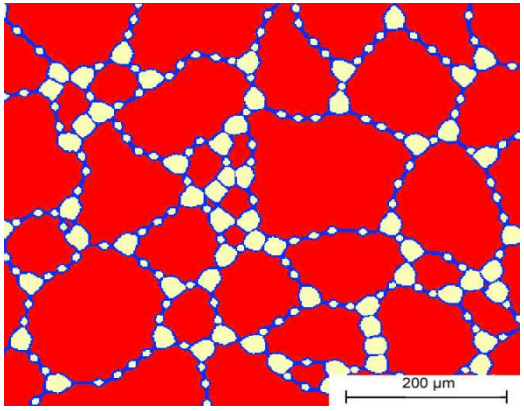
- Solidification (dendritic, cellular, peritectic, eutectic)
- Solid state reactions (grain growth, recrystallisation, phase transformations)
- Direct coupling to thermodynamic databases (contains TQ-interface*) or linear phase diagram approximation



multi-grain



1D, 2D or 3D



multiphase multicomponent

***from Thermo-Calc Software, Sweden**

The MICRESS® Story

1995: first microstructure simulations at ACCESS

1996: multi-phase-field model published (Physica D 94(1996), p.135-147.)

1999: simulations comprising thermodynamic databases

2003: MICRESS is commercially available

2005: MICRESS website is online: *www.micress.de*

2006: stress solver incorporated

2007: coupling to external temperature fields

2008: MICRESS user forum on website: www.micress.de/forum

2009: incorporation of nple and para-equilibrium models

2010: higher order terms for triple junctions etc.

2011: Version 6.0: 64bit Version with TQ

We…..the MICRESS group at Access:

Dr. Markus Apel

Dr. Bernd Böttger

Dr. Antoine Carre

Dr. Janin Eiken (formerly: J. Tiaden)

Dr. Georg J. Schmitz

Alexandre Viardin

Kathrin Graetz (master student)

New member: Ralph Altenfeld

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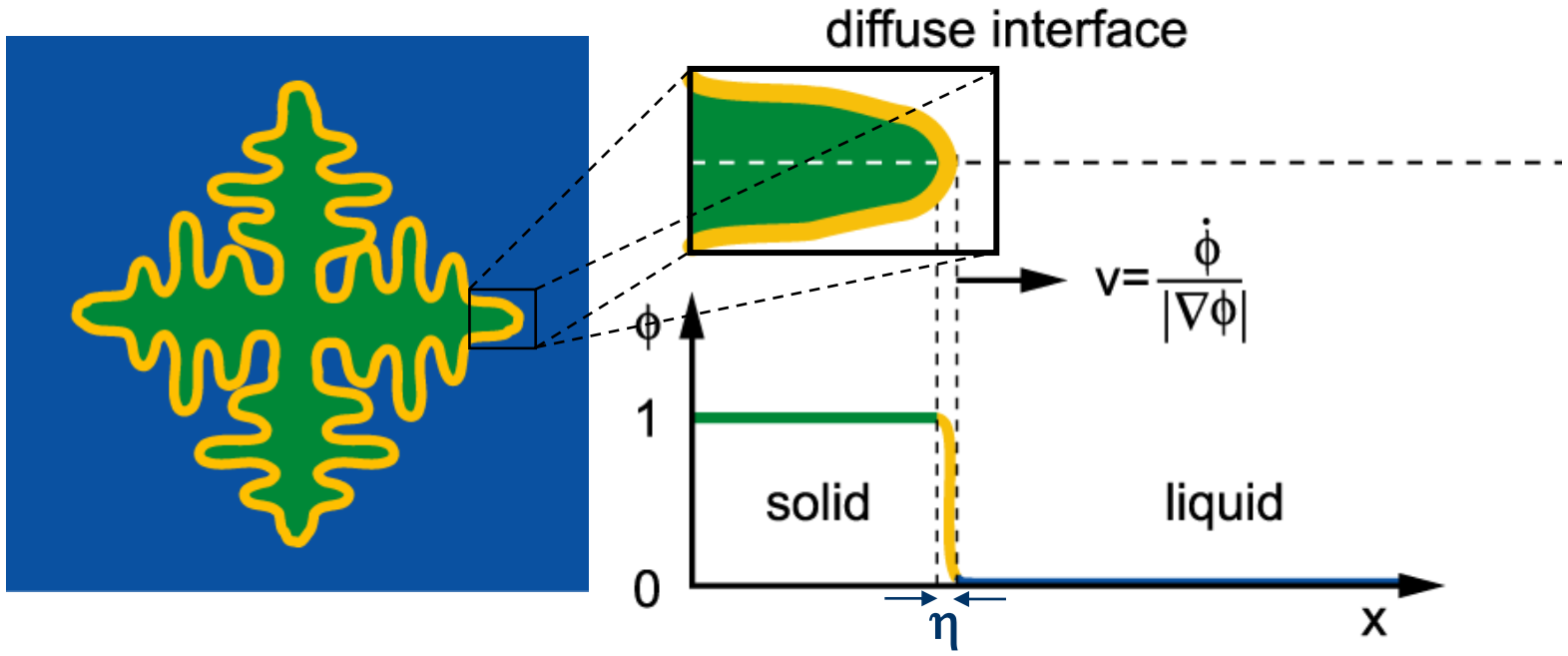
Phase-Field Model

- Diffuse interface, described by the phase-field parameter ϕ:



- The order parameter $\phi = \phi(x,t)$ corresponds to a density function for the phase state.
- η is the interface thickness (numerical parameter)

The Multiphase-Field Model

$$\{\phi_\alpha\}\ \alpha = 1 \ldots N$$

Vector order parameter

$$f = \sum_{\alpha \neq \beta} f_{\alpha\beta}(\{\phi_\alpha\}) + f_c$$

$f_{\alpha\beta}$: pair interaction energies

f_c : chemical free energy

$$= \sum_{\alpha,\beta} \frac{\sigma_{\alpha\beta}(\vec{n}_\alpha, \vec{n}_\beta)}{\eta_{\alpha\beta}} K^{\alpha\beta}(\Delta\phi_\alpha, \Delta\phi_\beta, \phi_\alpha, \phi_\beta) + \sum_\alpha \phi_\alpha f^\alpha(c_\alpha)$$

$$\Psi_{\alpha\beta} = \left(\frac{\delta}{\delta\phi_\alpha} - \frac{\delta}{\delta\phi_\beta} \right) f \qquad \dot{\phi}_\alpha = \sum_\beta \mu_{\alpha\beta} \Psi_{\alpha\beta}$$

$\psi_{\alpha\beta}$: interfacial growth operator

what is pragmatic?

- bulk thermodynamic data are used only for the chemical free energy f_c
- f^α is a function of c_α, not of c!

→ coupling to arbitrary thermodynamic databases possible!

Multiphase-Field Model: Phase-Field Equation

Multiphase-field equation:

$$\dot{\phi}_\alpha = \sum_\beta^n \mu^*_{\alpha\beta}\left[\sigma^*_{\alpha\beta}\left(\phi_\alpha \nabla^2\phi_\beta - \phi_\beta\nabla^2\phi_\alpha + \frac{\pi^2}{2\eta^2_{\alpha\beta}}(\phi_\alpha - \phi_\beta) + \sum_{\alpha\neq\beta\neq\gamma}^n J_{\alpha\beta\gamma}\right) + \frac{\pi}{\eta_{\alpha\beta}}\sqrt{\phi_\alpha\phi_\beta}\,\Delta G_{\alpha\beta}\right]$$

dual interface terms "double_obstacle"

higher interface terms "multi_obstacle"

chemical driving force

$\eta_{\alpha\beta}$ = interface thickness

$\mu_{\alpha\beta}$ = interfacial mobility (anisotropic)

$\sigma_{\alpha\beta}$ = interfacial energy (anisotropic)

$\Delta G_{\alpha\beta}$ = driving force

- *Steinbach et al; Physica D 1996*
- *Tiaden et al. Physica D 1998*
- *Steinbach, Pezzolla; Physica D 1999*
- *Eiken, Böttger, Steinbach; Phys. Rev. E 2006*

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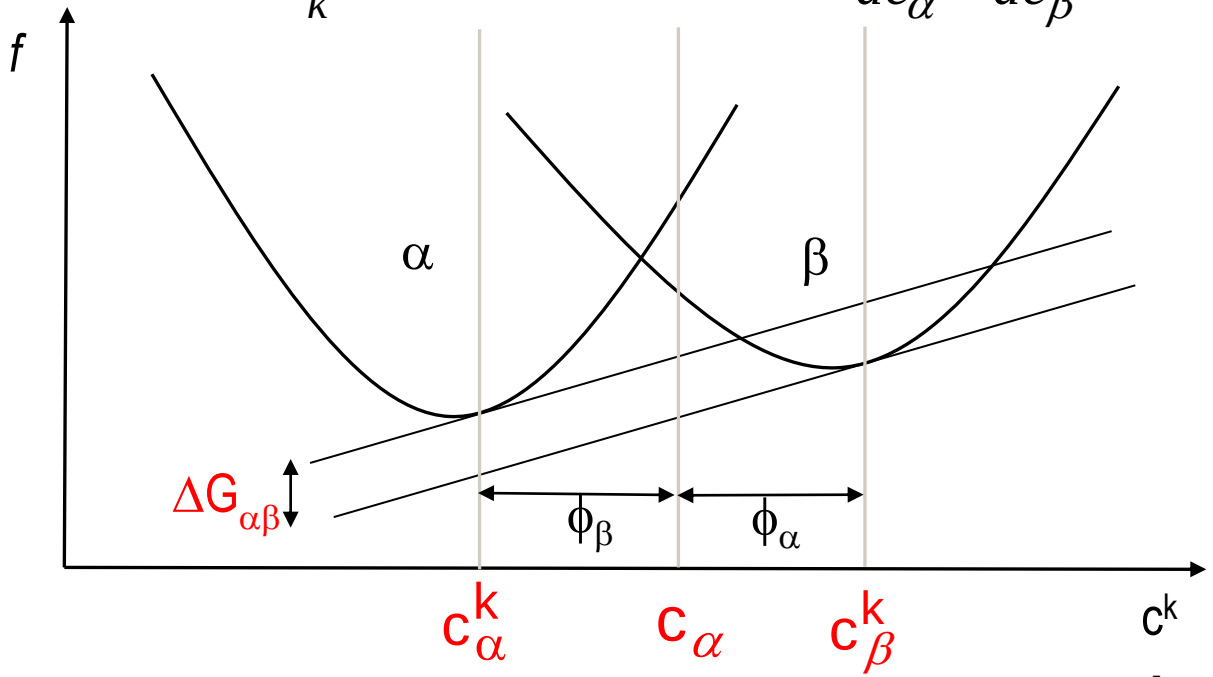
Phase-Field and Thermodynamics: Quasi-Equilibrium

- minimization of the chemical free energy $f_c = \sum_\alpha \phi_\alpha f_\alpha$ at constant phase fractions ϕ_α gives:

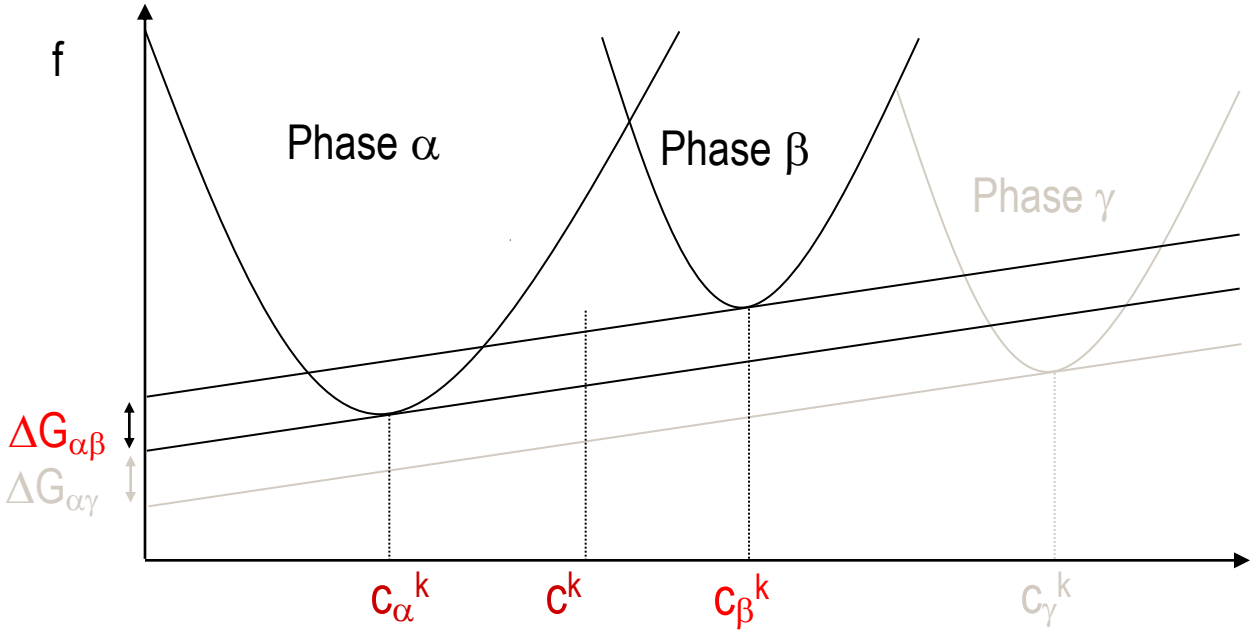
$$\Delta G_{\alpha\beta} = f_\alpha - f_\beta + \sum_k \tilde{\mu}^k \left(c_\alpha^k - c_\beta^k \right) \quad , \quad \tilde{\mu}^k = \frac{df_\alpha}{dc_\alpha^k} = \frac{df_\beta}{dc_\beta^k}$$



- $\Delta G_{\alpha\beta}$, c_α^k and c_β^k are calculated iteratively including the mass balance: $\phi_\alpha c_\alpha^k + \phi_\beta c_\beta^k = c^k$

Phase-Field and Thermodynamics: Multiphase Quasi-Equilibrium

- additional phases are included into the iteration process:



- iteration for N phases:

$$\Delta G_{\alpha\beta} = f_\alpha - f_\beta + \sum_k \tilde{\mu}^k \left(c_\alpha^k - c_\beta^k \right) \quad , \quad \tilde{\mu}^k = \frac{df_\alpha}{dc_\alpha^k} = \frac{df_\beta}{dc_\beta^k} = \frac{df_\gamma}{dc_\gamma^k} \ldots, \qquad \sum_i \phi_i \, c_i^k = c^k$$

➡ consistent quasi-equilibria for all phase pairs

➡ problem: **huge calculation times!**

Phase-Field and Thermodynamics: Multi-Binary Extrapolation

- driving-force:

$$\Delta G^{*}_{\alpha\beta} = \Delta G_{\alpha\beta} + \sum_k \left(\frac{\partial \Delta G_{\alpha\beta}}{\partial c^k_\alpha} \right)_T \Delta c^k_\alpha + \left(\frac{\partial \Delta G_{\alpha\beta}}{\partial T} \right)_{c^k_\alpha} \Delta T$$

- condition for extrapolation: $\Delta G_{\alpha\beta} = \Delta G_{\beta\alpha}$

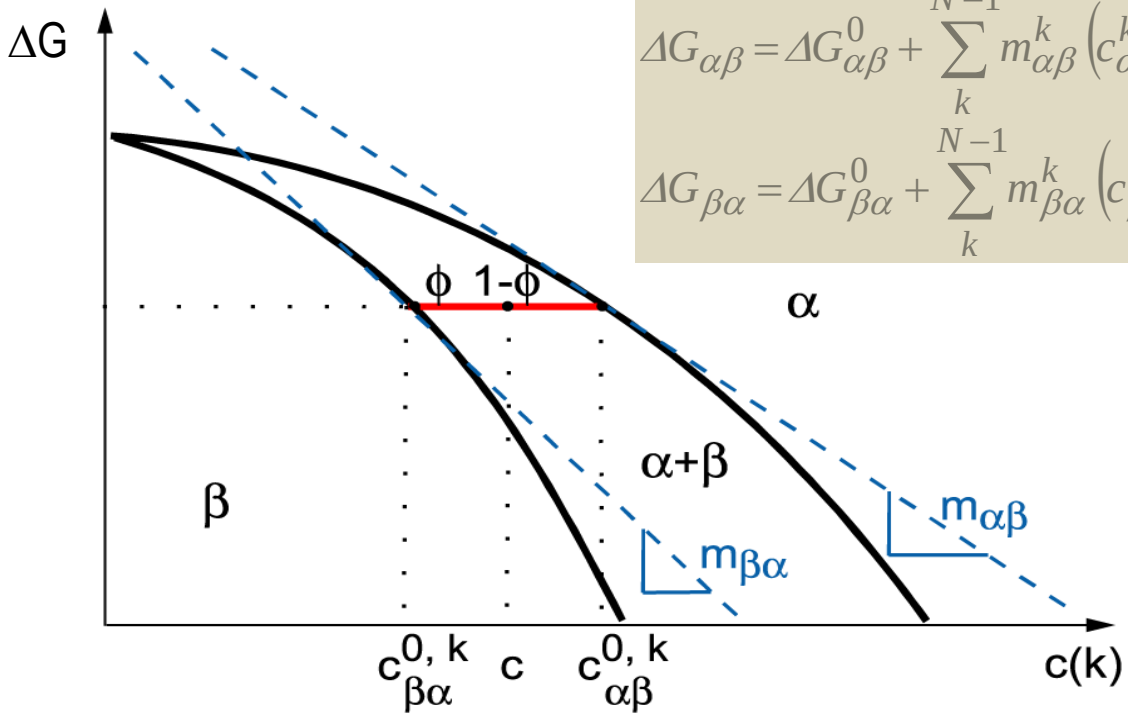
$$m^k_{\alpha\beta} = \left(\frac{\partial \Delta G_{\alpha\beta}}{\partial c^k_\alpha} \right)_T, \quad m^k_{\beta\alpha} = \left(\frac{\partial \Delta G_{\alpha\beta}}{\partial c^k_\beta} \right)_T$$

$$c^{0,k*}_{\alpha\beta} = c^{0,k}_{\alpha\beta} + \left(\frac{\partial c^k_\alpha}{\partial T} \right)_{c^{l\neq k}_\alpha} dT$$

$$c^{0,k*}_{\beta\alpha} = c^{0,k}_{\beta\alpha} + \left(\frac{\partial c^k_\beta}{\partial T} \right)_{c^{l\neq k}_\beta} dT$$

$$c^k_\alpha = \frac{c^k - \sum_\gamma \phi_\gamma \left(c^{0,k*}_{\gamma\alpha} - c^{0,k*}_{\alpha\gamma} \, m^k_{\gamma\alpha} / m^k_{\alpha\gamma} \right)}{\sum_\gamma \phi_\gamma \, m^k_{\gamma\alpha} / m^k_{\alpha\gamma}}$$

$$c^k_\beta = \frac{c^k - \sum_\gamma \phi_\gamma \left(c^{0,k*}_{\gamma\beta} - c^{0,k*}_{\beta\gamma} \, m^k_{\gamma\beta} / m^k_{\beta\gamma} \right)}{\sum_\gamma \phi_\gamma \, m^k_{\gamma\beta} / m^k_{\beta\gamma}}$$



$$\Delta G_{\alpha\beta} = \Delta G^0_{\alpha\beta} + \sum_k^{N-1} m^k_{\alpha\beta} \left(c^k_\alpha - c^{0,k}_{\alpha\beta} \right)$$

$$\Delta G_{\beta\alpha} = \Delta G^0_{\beta\alpha} + \sum_k^{N-1} m^k_{\beta\alpha} \left(c^k_\beta - c^{0,k}_{\beta\alpha} \right)$$

➡ considerably faster!

Eiken, Böttger, Steinbach; Phys. Rev. E 2006

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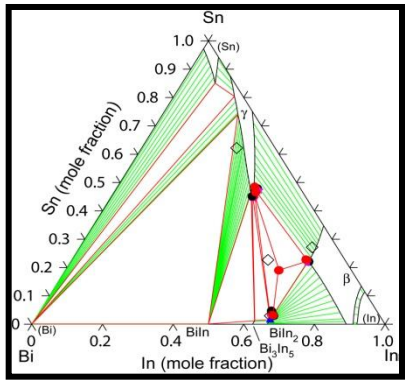
Use of Thermodynamic Data in MICRESS®



CALPHAD database

Thermo-Calc

TQ-Interface

nucleation undercooling

driving force

element redistribution

diffusion matrix

enthalpy

MICRESS®

time loop

nucleation model

$\Delta T_{und} > \Delta T_{crit}$?

multiphase-field solver

$\dot{\phi}_\alpha(x,t) = \sum_\beta \mu_{\alpha\beta}(\sigma_{\alpha\beta}K + w\Delta G_{\alpha\beta})$

multicomponent diffusion solver

$\dot{\vec{c}}(x,t) = \nabla \sum_\alpha \phi_\alpha \vec{\vec{D}}_\alpha \nabla \vec{c}_\alpha$

temperature solver

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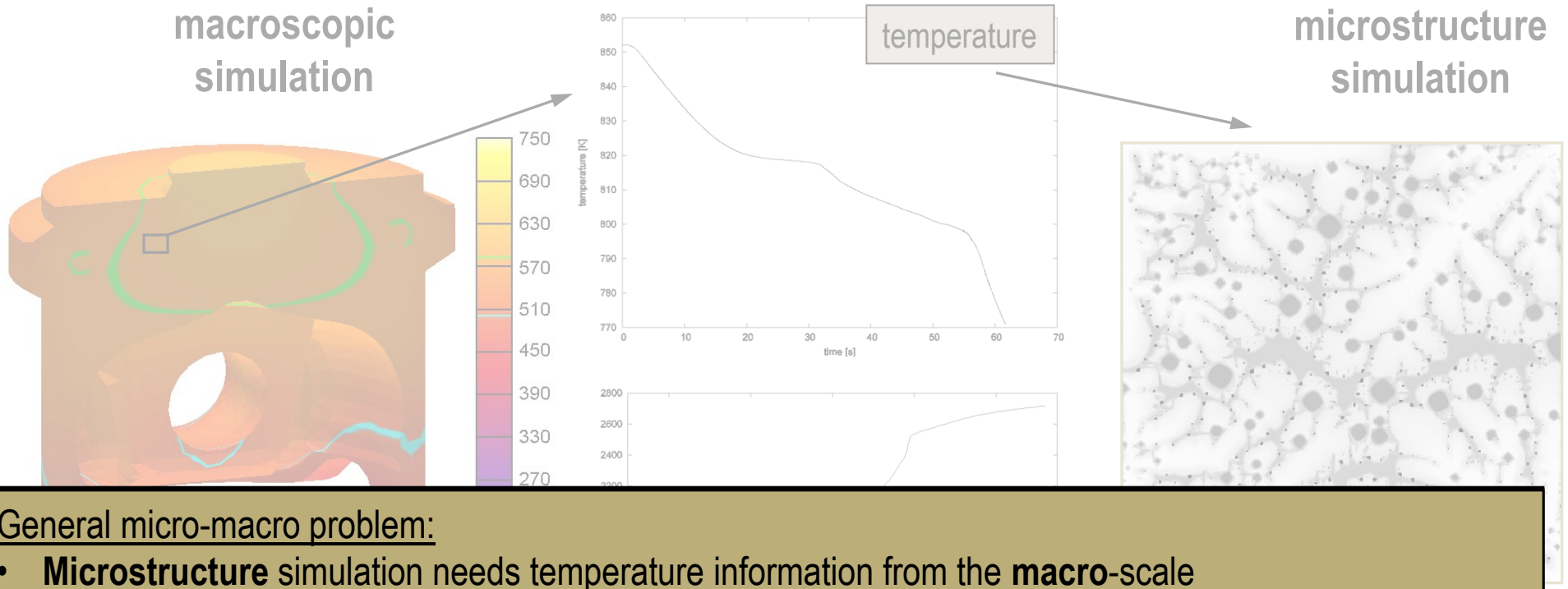
Linking to the Process: The General Micro-Macro Problem



General micro-macro problem:

- **Microstructure** simulation needs temperature information from the **macro**-scale
- **Macroscopic** simulation needs latent heat effects from the **micro**-scale

→ Exact solution would require microstructure simulation on the **whole** casting!

→ Which approximations are reasonable?

Linking to the Process: The General Micro-Macro Problem

Typical approximations for phase-field simulation:

- no latent heat is taken into account
  - e.g. ripening, grain growth
  - slow processes (e.g. solid-solid)
  - high temperature gradient (Bridgman process)
- global temperature effect (G=0)
  - slow processes in thermally isolated materials
  - small samples (DTA)
- temperature is solved on different scale (e.g. free growing dendrite)
  - special assumptions are needed

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“Bridgman” Approximation

Bridgman Apparatus:

-large constant thermal gradient
-pulling velocity is controlled
→ T gradient and cooling rate practically are independent!

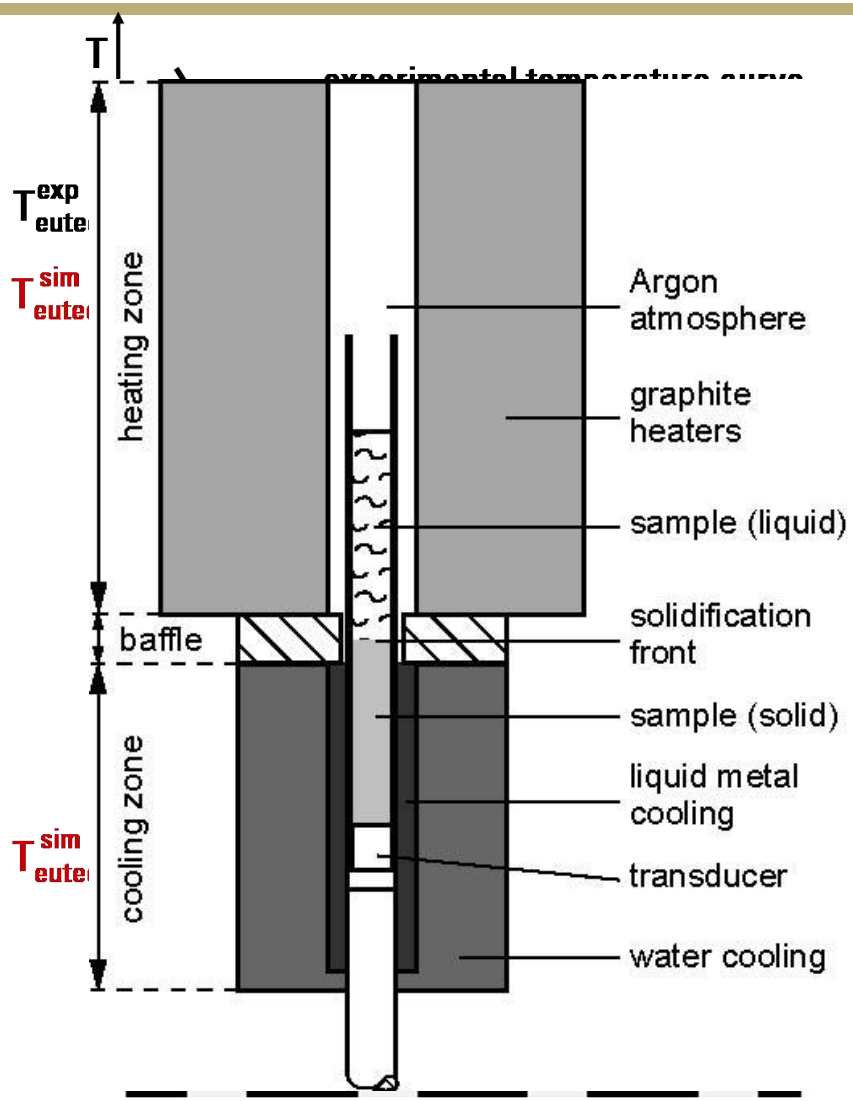
“Bridgman” Approximation:

- T gradient and cooling rate are regarded as independent external parameters for microstructure simulation
- are taken from experiments or process simulation results

Problem with Approximation:

- thermal conditions may be not consistent with microstructure formation

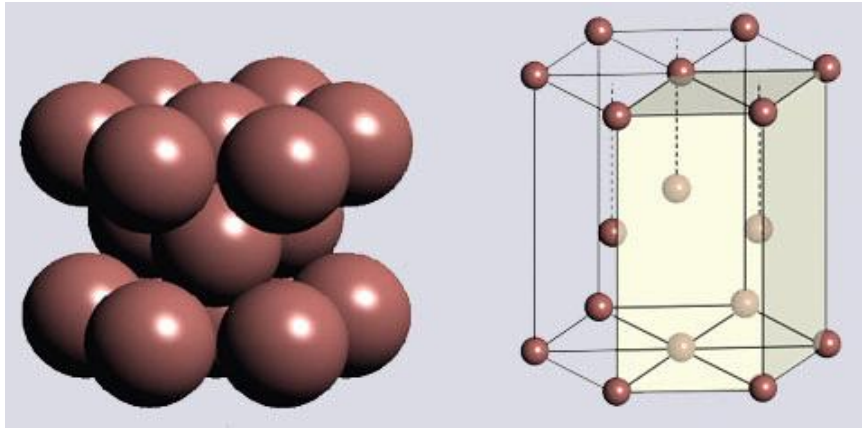
→ “violation” of microstructure



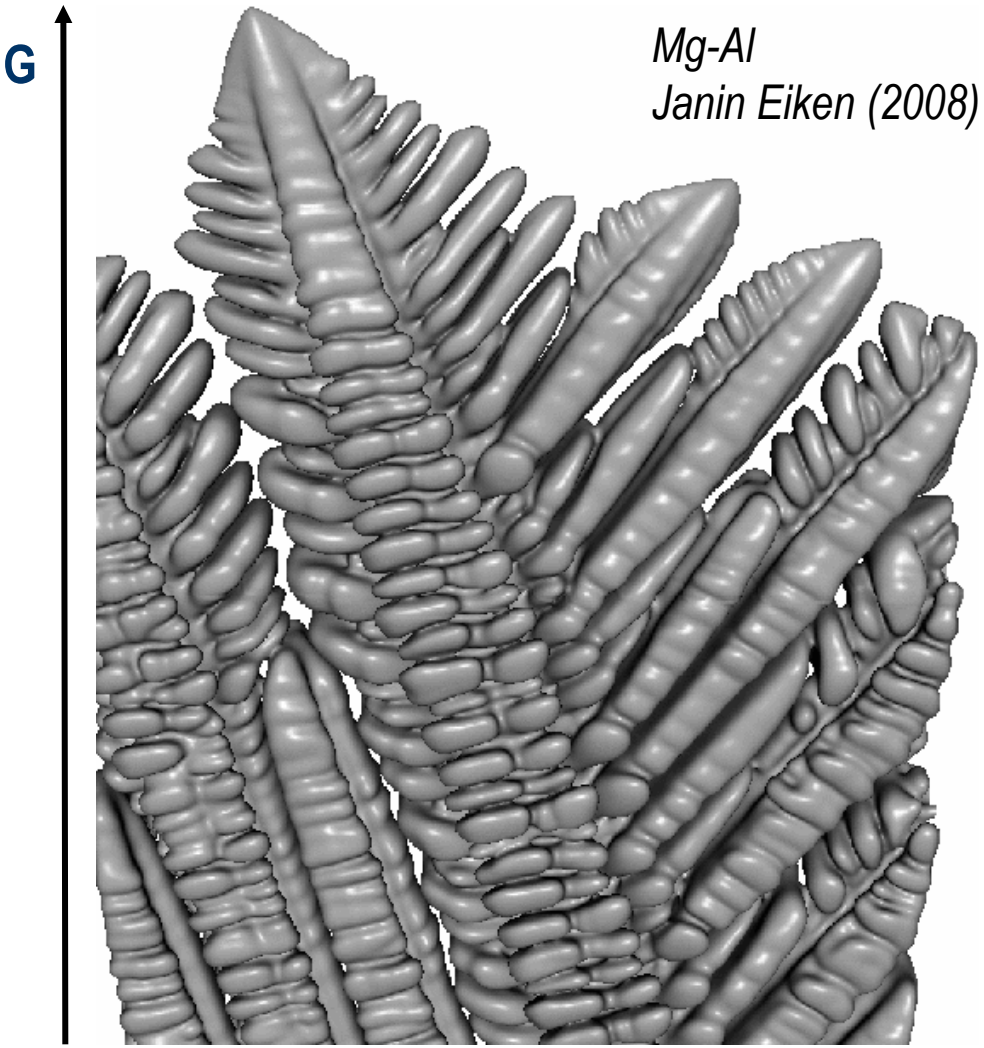
2D Representations of Directional Dendritic Growth

- 3D simulations are possible with MICRESS®, but need a high computational effort. At present, 3D is not realistic for:
  - multicomponent technical alloy
  - simulation of complete solidification (evtl. with precipitation of secondary phases)

⇨ Simulation of reasonable 2D projections!



hexagonal symmetry of the crystal lattice



2D Representations of Directional Dendritic Growth: Longitudinal Projection

a) longitudinal projection

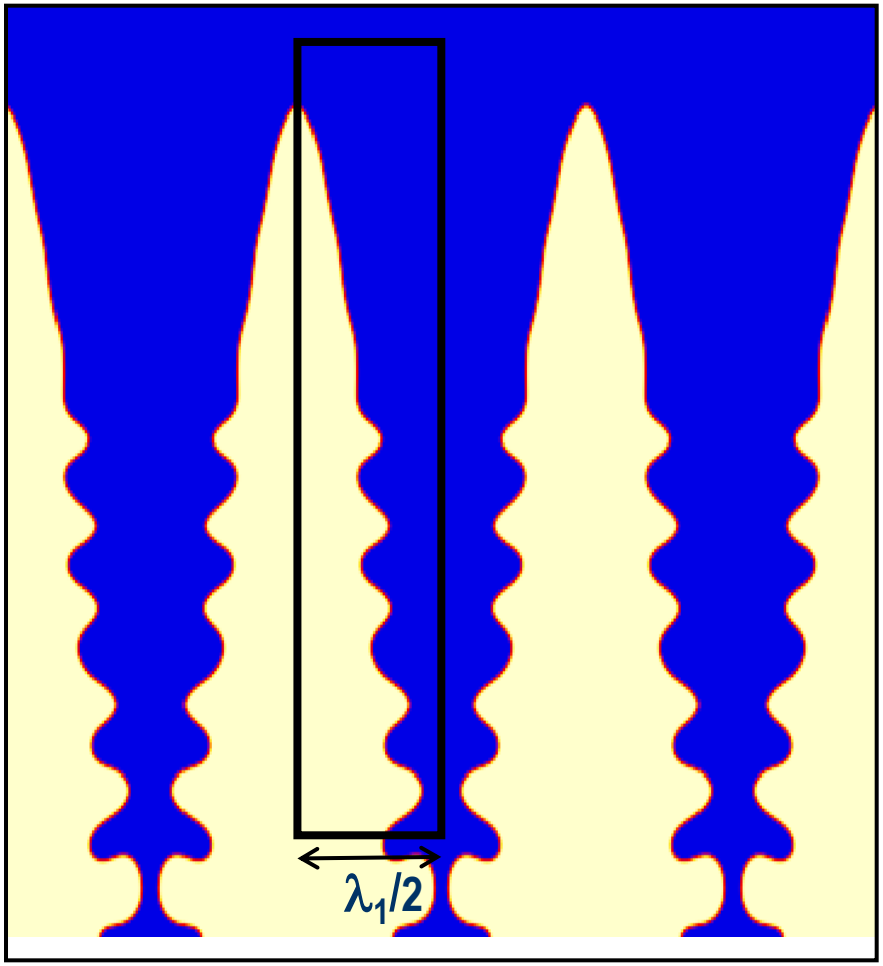
define T-gradient in z-direction and cooling rate

```
…
# Initial temperature at the bottom?  (real)  [K]
1660.000
# Temperature gradient in z-direction?  [K/cm]
50.0000
# Cooling rate? [K/s]
-2.5000
…
```

smallest unit cell is ½ dendrite with symmetric boundary conditions

```
# Boundary conditions for phase field in each direction
# Options: i (insulation) s (symmetric) p (periodic/wrap-around)
#          g (gradient)   f (fixed)     w (wetting)
# Sequence: E W (N S, if 3D) B T borders
ssii
#
# Boundary conditions for concentration field in each direction
# Options: i (insulation) s (symmetric) p (periodic/wrap-around) g
(gradient) f (fixed)
# Sequence: E W (N S, if 3D) B T borders
ssii
```

initial seed at lower left corner

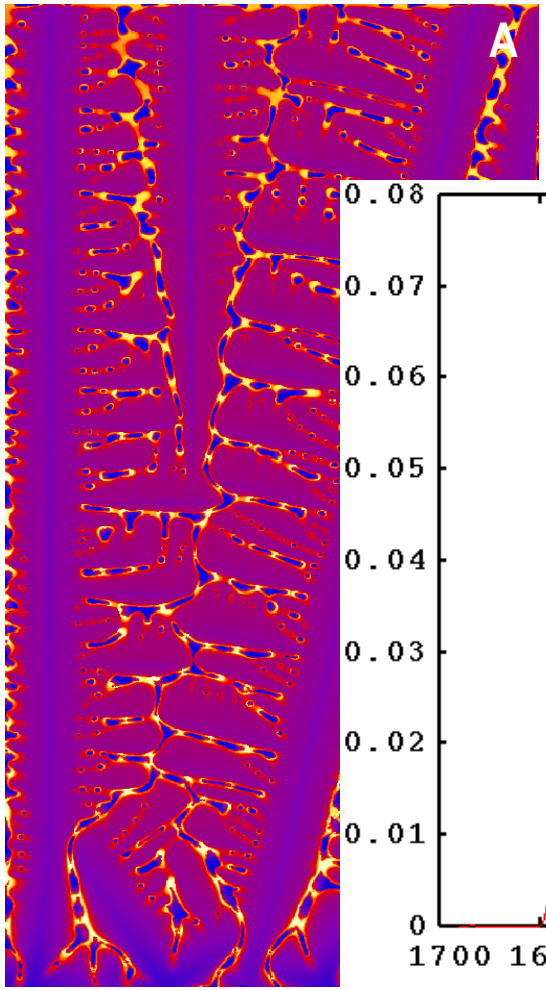


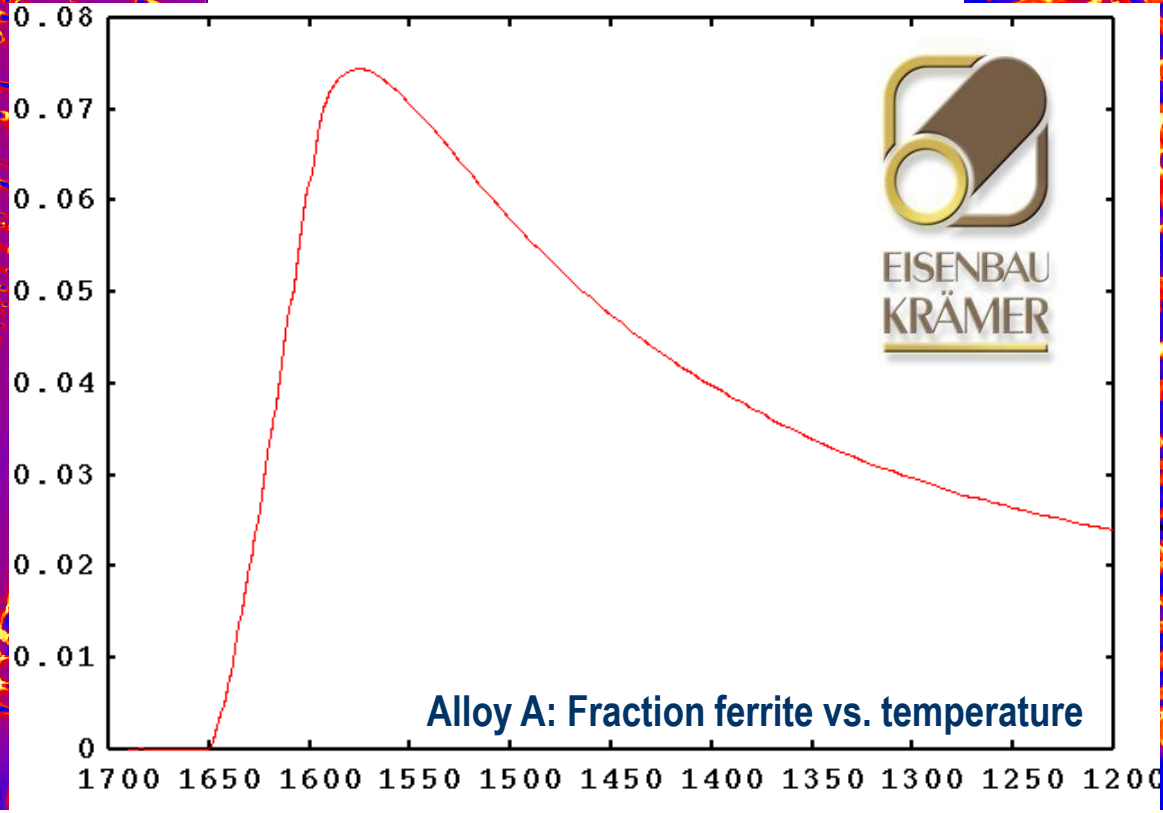
Example 1:

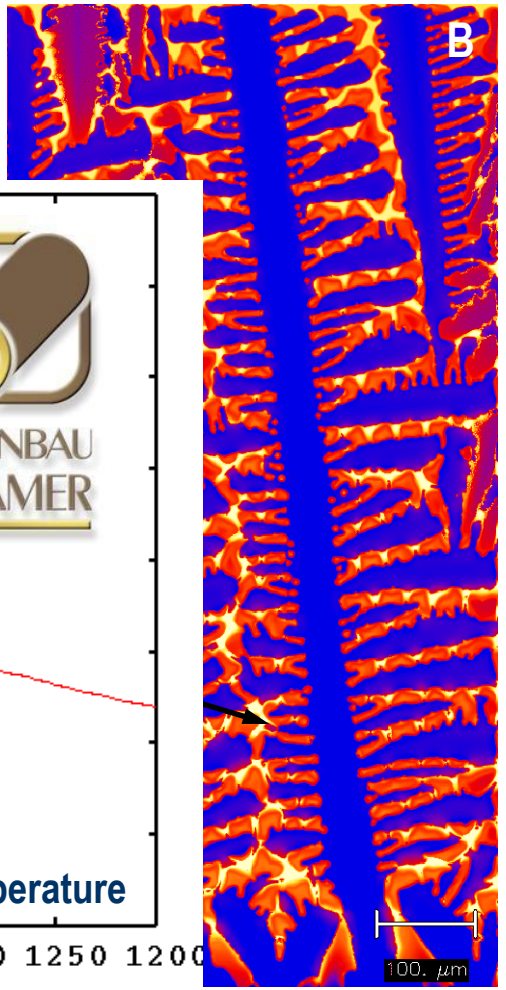
Solidification of Stainless Steel

Solidification of Stainless Steel

	Cr	Ni	Mn	Mo	Si	P	C	N
wt%	17.0	12.0	2.0	1.5	0.75	0.05	0.03	0.01







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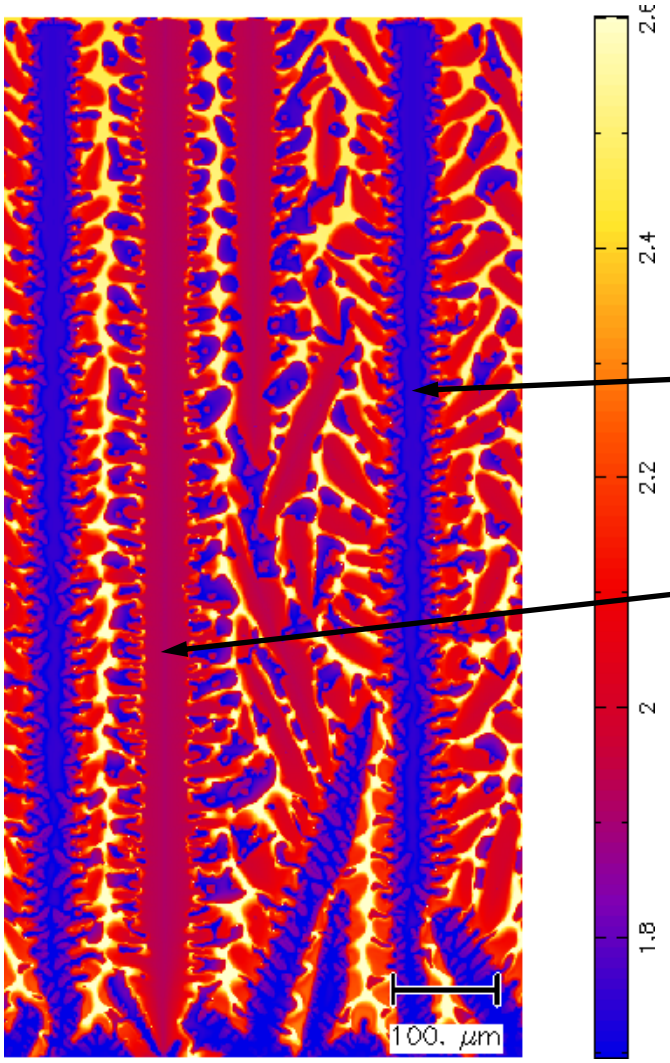
Solidification of Stainless Steel



	Cr	Ni	Mn	Mo	Si	P	C	N
wt%	17.0	9.5	2.0	1.5	0.75	0.05	0.03	0.01

ferrite

austenite

→MICRESS® is an excellent tool for alloy development!

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Example 2:

Solidification and Heat Treatment of a Technical Ni-Base Superalloy

(removed for confidentiality)

Example 3:

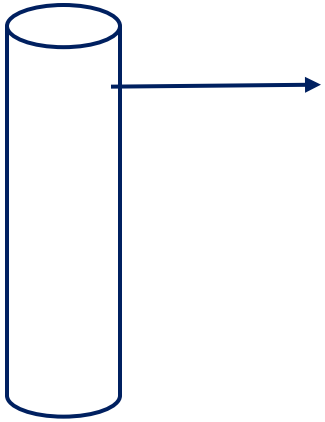
Directional Solidification of CMSX-4

Directional Solidification of CMSX-4

Average composition for simulation:

element	Cr	Co	Mo	W	Ta	Al	Ti	Re	Hf
wt %	6,5	9	0,6	6	6,5	5,6	1	3	0,1

Casting of cylindrical geometry using a Bridgman furnace

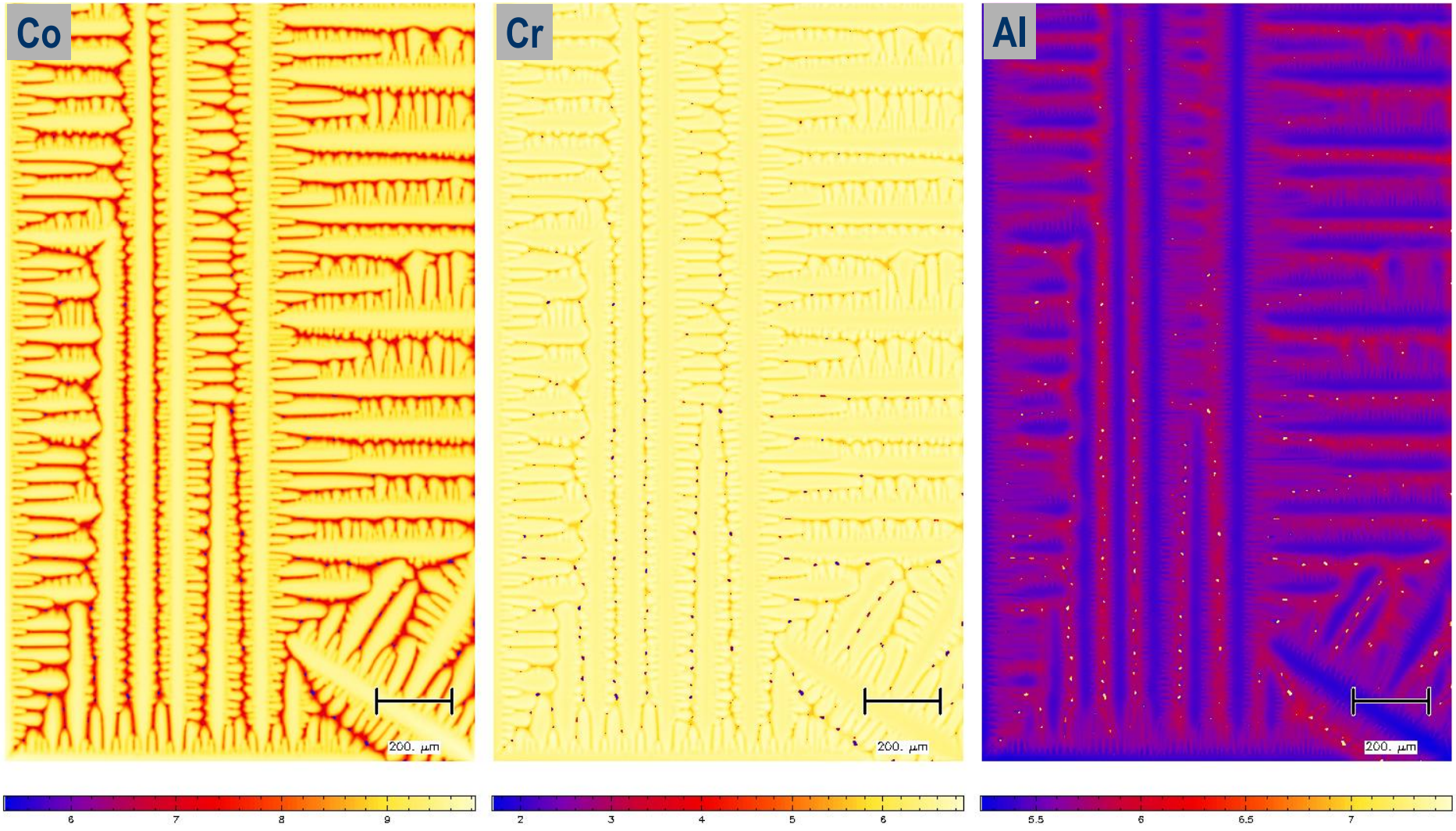


v [mm/min]	8,6
G [K/mm]	4,5
λ [µm]	199

Thermodynamic database: TTNI7

Mobility database: MOBNI for diffusion in fcc (incl. cross terms)

Directional Solidification of CMSX-4



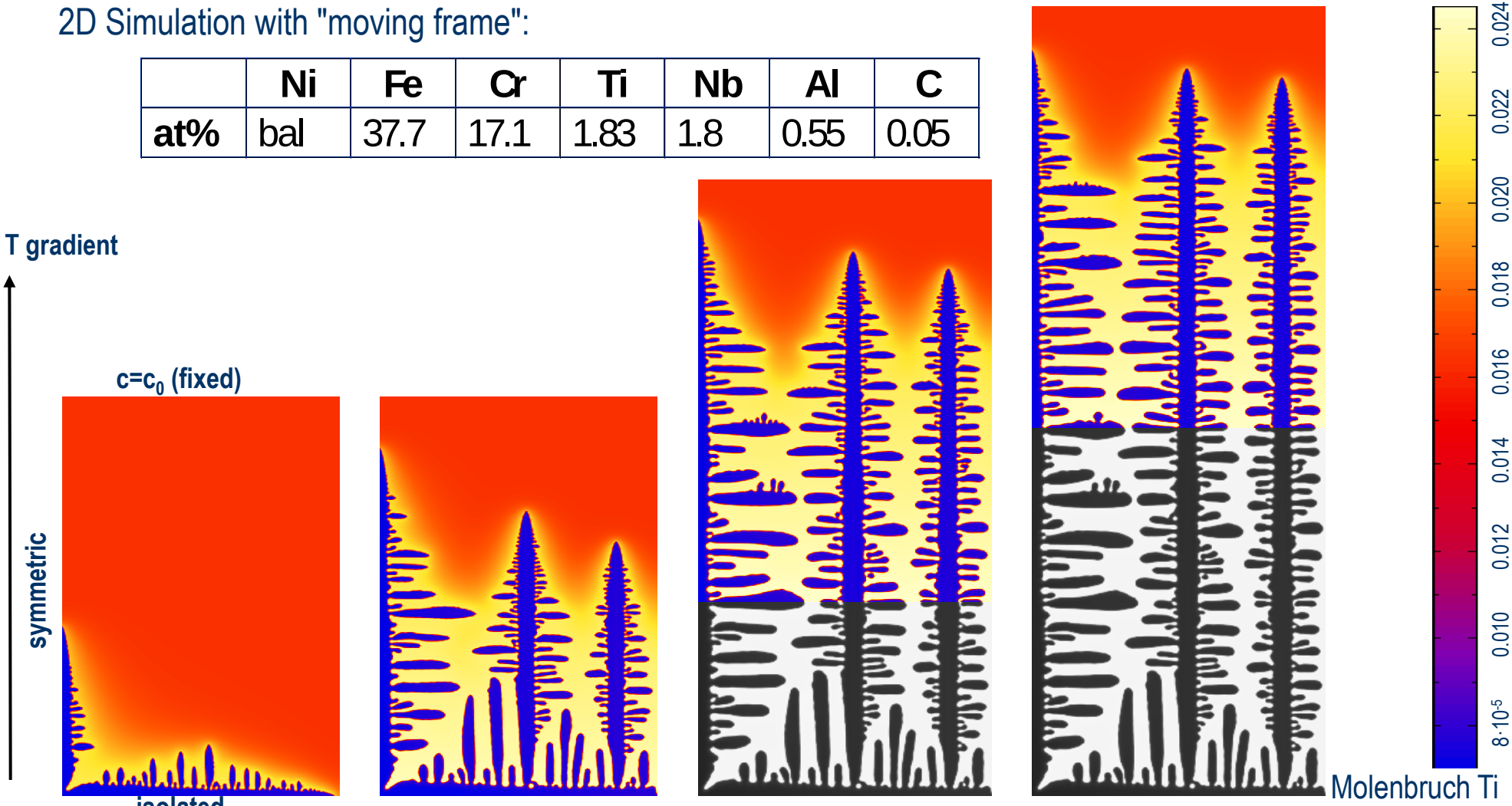
Example 4:

Remelting of IN706 – Moving Frame

Remelting of IN706 – Moving Frame

2D Simulation with "moving frame":

	Ni	Fe	Cr	Ti	Nb	Al	C
at%	bal	37.7	17.1	1.83	1.8	0.55	0.05



2D Representations of Directional Dendritic Growth: Transversal Isothermal Projection

b) transversal isothermal projection

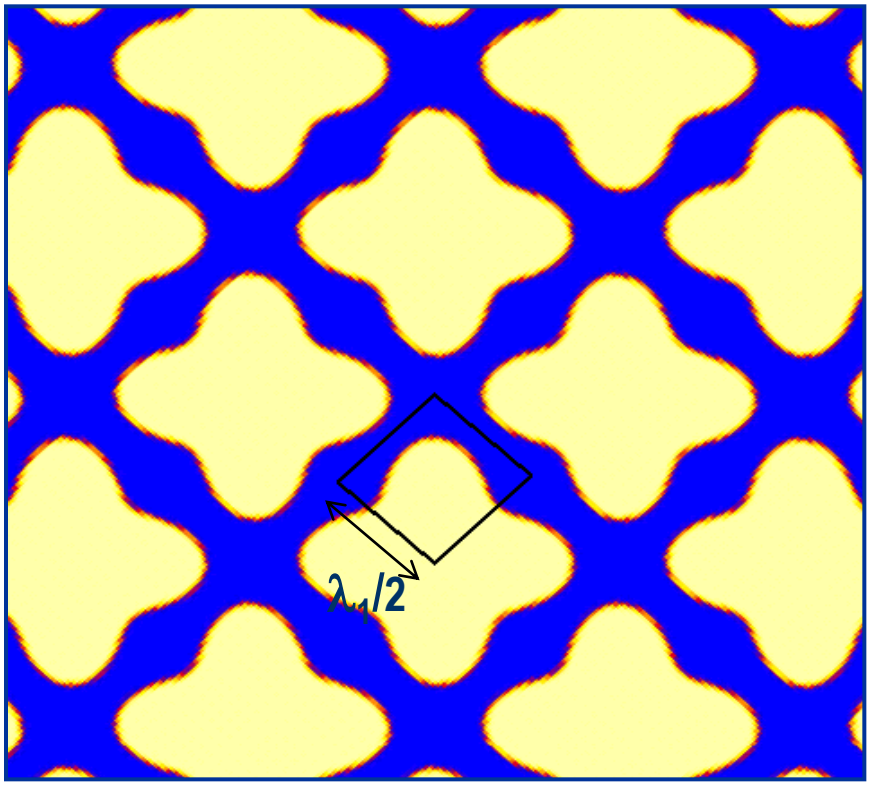
define cooling rate without T-gradient

```
…
# Initial temperature at the bottom?  (real)  [K]
1660.000
# Temperature gradient in z-direction?  [K/cm]
0.0000
# Cooling rate? [K/s]
-2.5000
…
```

smallest unit cell is ¼ dendrite with symmetric boundary conditions

```
# Boundary conditions for phase field in each direction
# Options: i (insulation) s (symmetric) p (periodic/wrap-around)
#          g (gradient)   f (fixed)     w (wetting)
# Sequence: E W (N S, if 3D) B T borders
ssss
#
# Boundary conditions for concentration field in each direction
# Options: i (insulation) s (symmetric) p (periodic/wrap-around) g
(gradient) f (fixed)
# Sequence: E W (N S, if 3D) B T borders
ssss
```

quadratic domain with initial seed at lower left corner



Example 5:

ESU Solidification of IN718

(removed for confidentiality)

ESU Solidification of IN718: Array with Grain Boundary

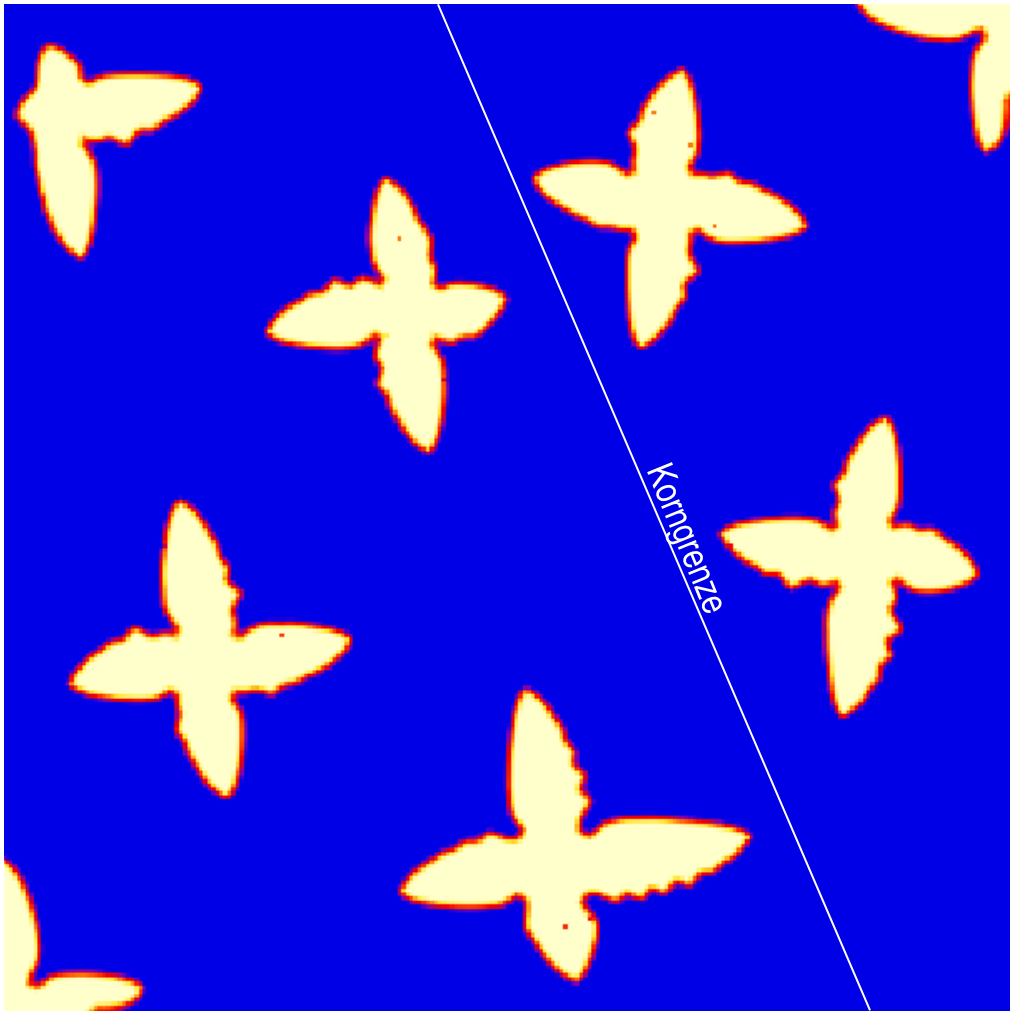
- simulation domain: 500 x 500 µm

- grid resolution: 2 µm

- 2 grains with regular array of different orientations

→ more realistic

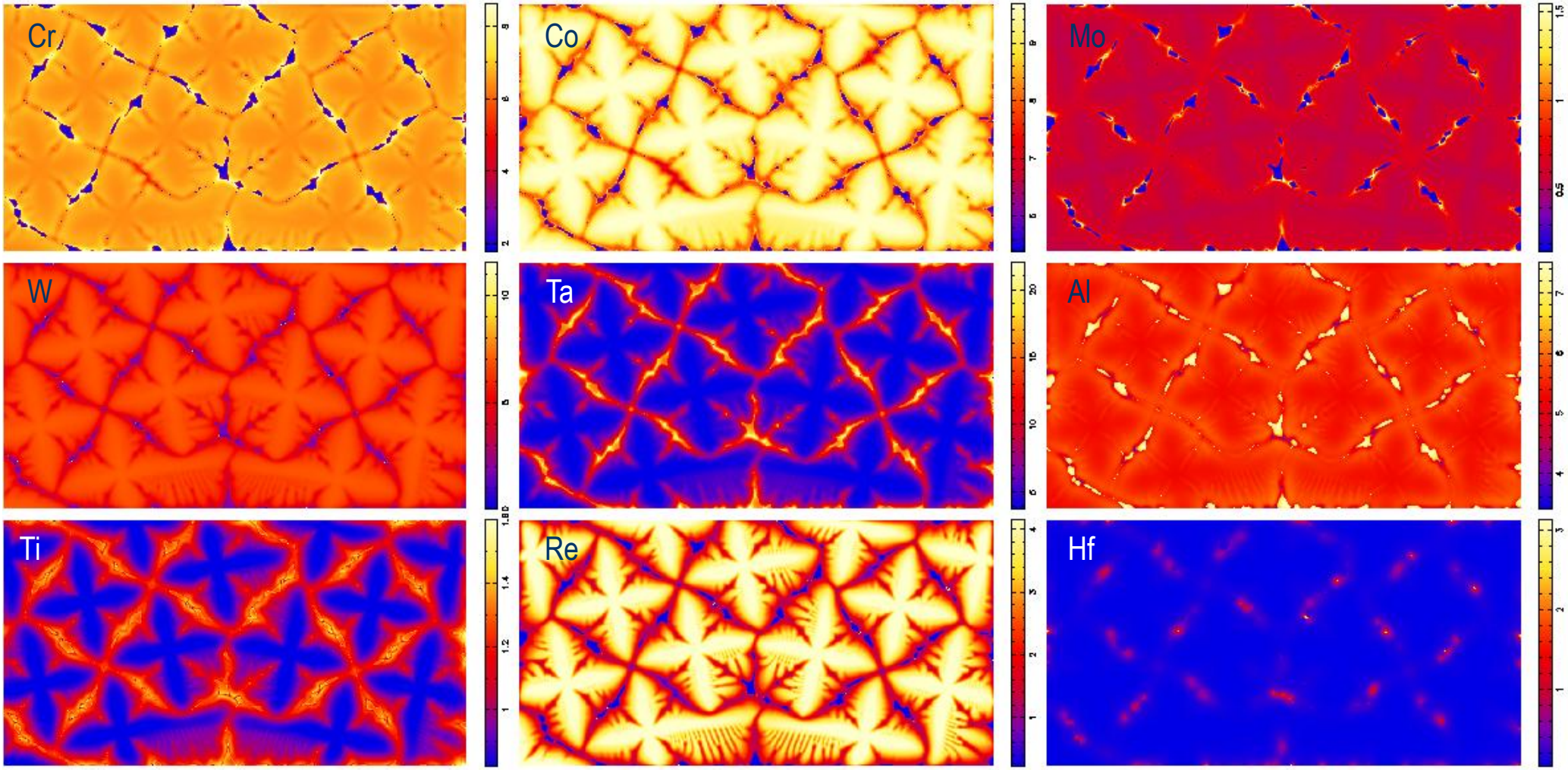
→improved statistics on phase fractions etc.



Example 6:

CMSX-4: continued

CMSX-4: continued



Outline

1. Introduction
2. Pragmatic Multi-Phase-Field Model
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4. **Simulation of Technical Alloys and Processes: Examples**
    a) Linking to the Process: The General Micro-Macro Problem
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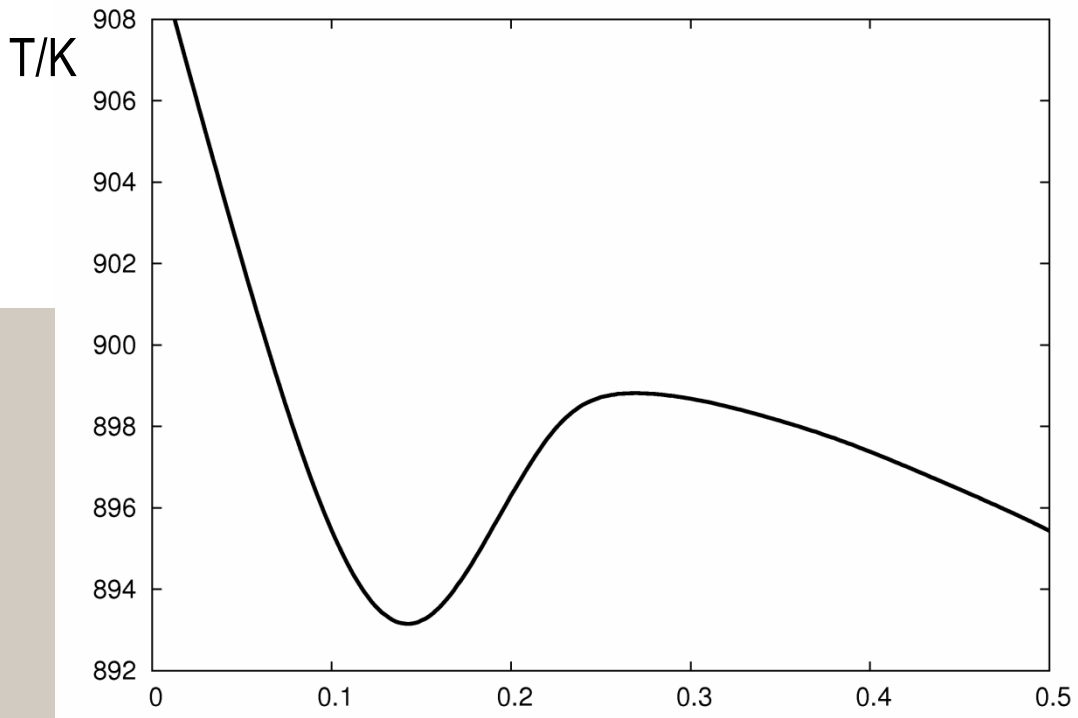
5. Conclusion

“DTA” Approximation

DTA apparatus:

- very small samples, no temperature gradient
- surrounding temperature is controlled

→ temperature of sample is results of balance between heat flux and latent heat



“DTA” approximation:

- no temperature gradient
- global heat extraction rate
- temperature is calculated from heat balance

$$\dot{q}dt = \frac{1}{V}\int_V \sum_\alpha d\left(H_\alpha \phi_\alpha\right) dV$$

Problem with approximation:

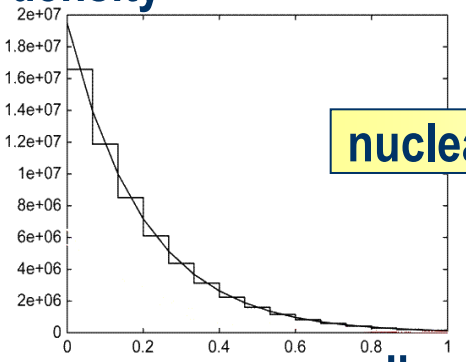
- no problems with consistency of temperature with microstructure, but

→ huge unrealistic recalescence

Example 7:

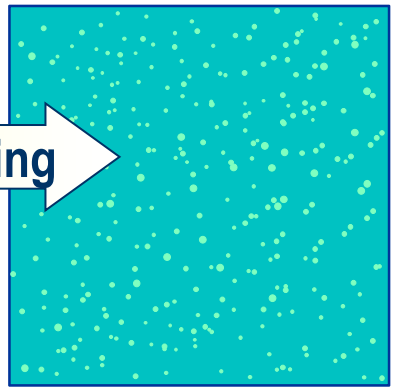
Grain Size of Magnesium Alloys AZ31, AZ61, AZ91

Grain Size of Magnesium Alloys AZ31, AZ61, AZ91: Nucleation Modell



nucleant distribution

nucleant positioning



nucleants with different radii

Nucleation-Model

$\Delta T_{crit}(r) < \Delta T(\vec{c}, T)$?

critical undercooling

new nucleus

Multi-Phase-Field-Solver

Multicomponent Diffusion-Solver

Temperature-Solver

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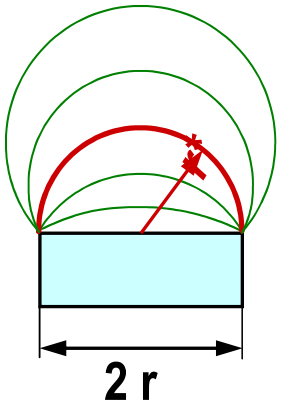
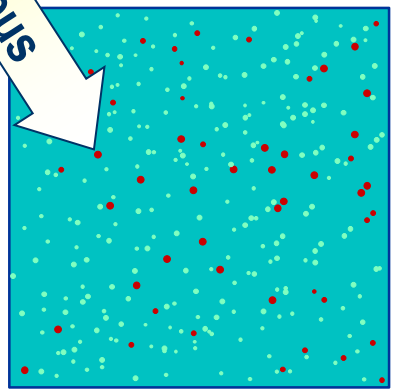


$$\Delta T_{crit}(r) = \frac{2\sigma}{\Delta S \cdot r}$$



nuclei

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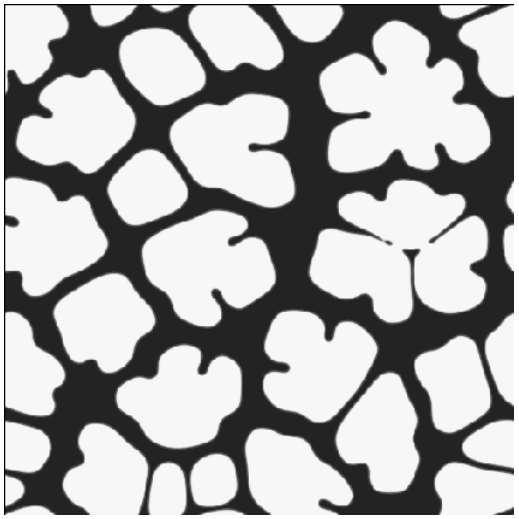
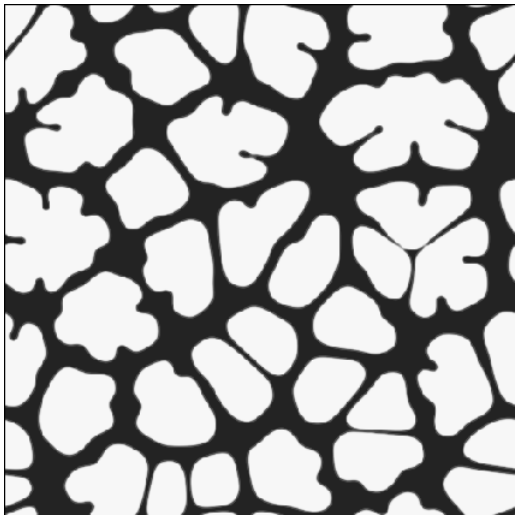
Grain Size of Magnesium Alloys AZ31, AZ61, AZ91

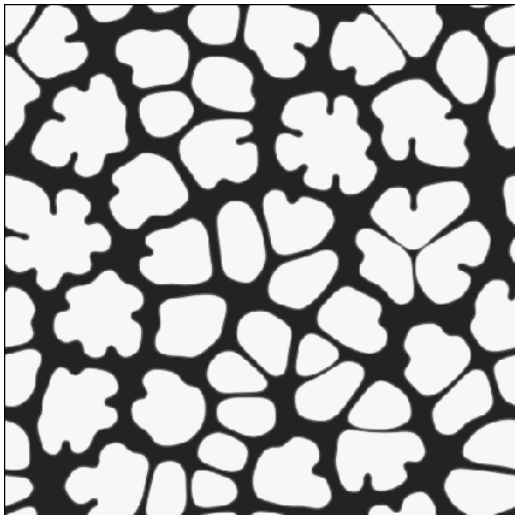
Mg-3%Al-1%Zn



Mg- 6%Al-1%Zn



Mg- 9%Al-1%Zn

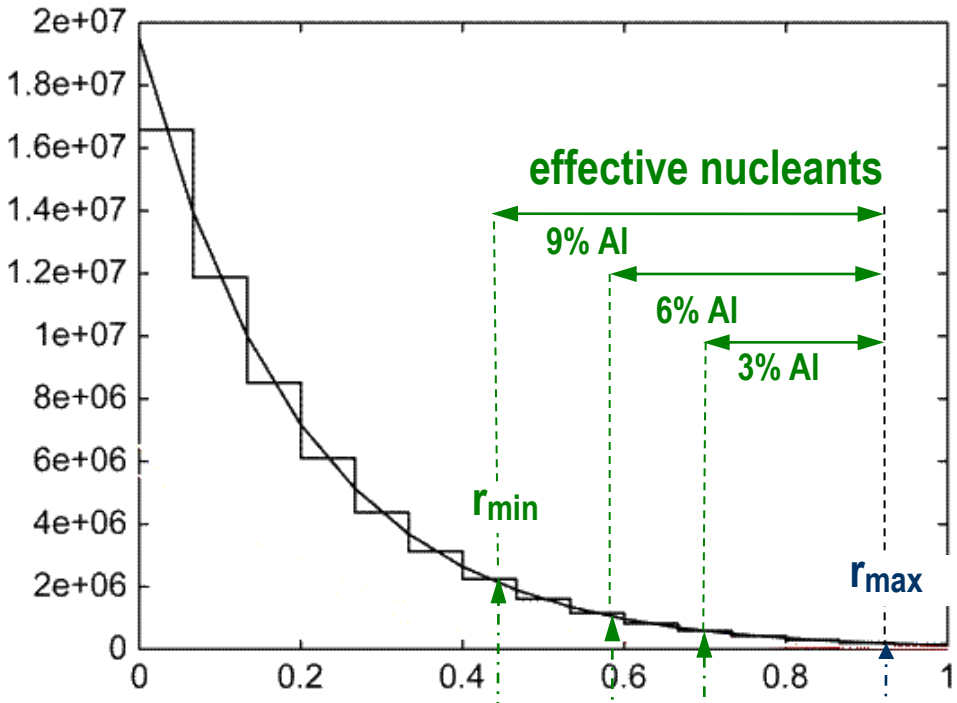


increased aluminium content

AZ31 → AZ91

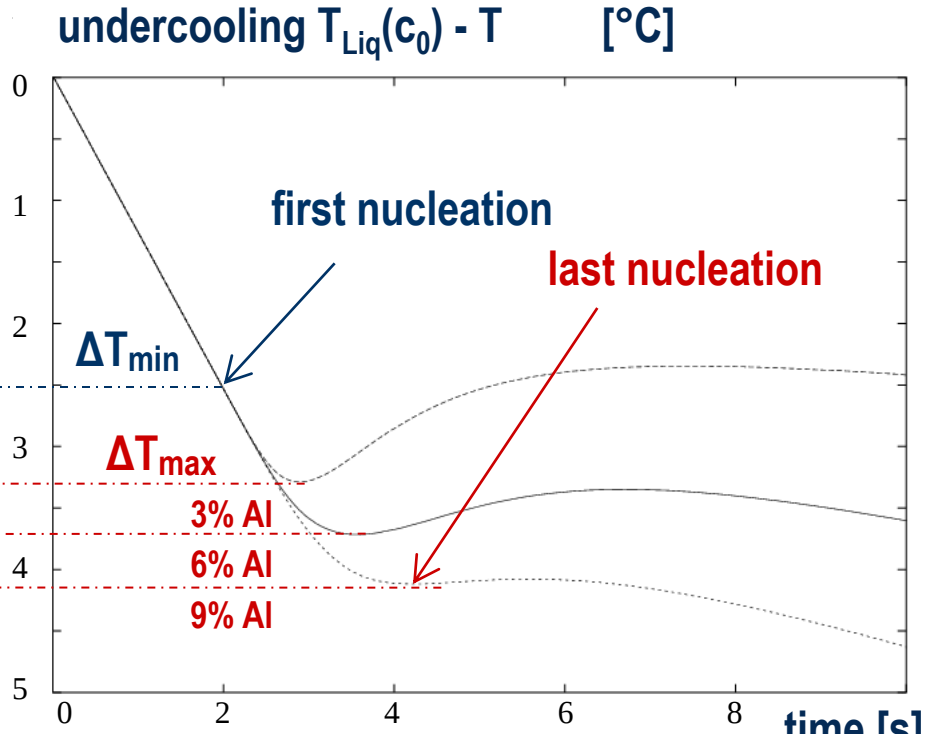
decreased grain size

Grain Size of Magnesium Alloys AZ31, AZ61, AZ91: Nucleation Modell



$$r = \frac{2\sigma}{\Delta S \cdot \Delta T}$$

undercooling



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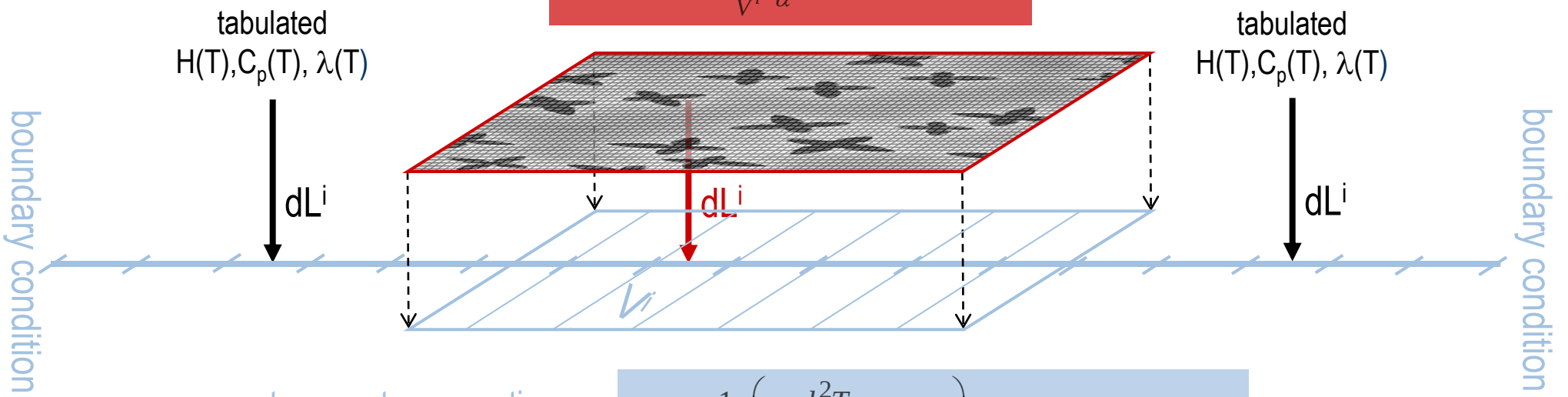
Multiphase-Field Model with Integrated 1D Temperature Solver

$$H^i(T^i) = \frac{1}{V^i}\int_{V^i}\sum_{\alpha}\left(H_\alpha(T^i)\phi_\alpha\right)dV$$

$$C_p{}^i(T^i) = \frac{1}{V^i}\int_{V^i}\sum_{\alpha}\left(C_{p,\alpha}(T^i)\phi_\alpha\right)dV$$

$$\lambda^i(T^i) = \frac{1}{V^i}\int_{V^i}\sum_{\alpha}\left(\lambda_\alpha(T^i)\phi_\alpha\right)dV$$

CALPHAD database

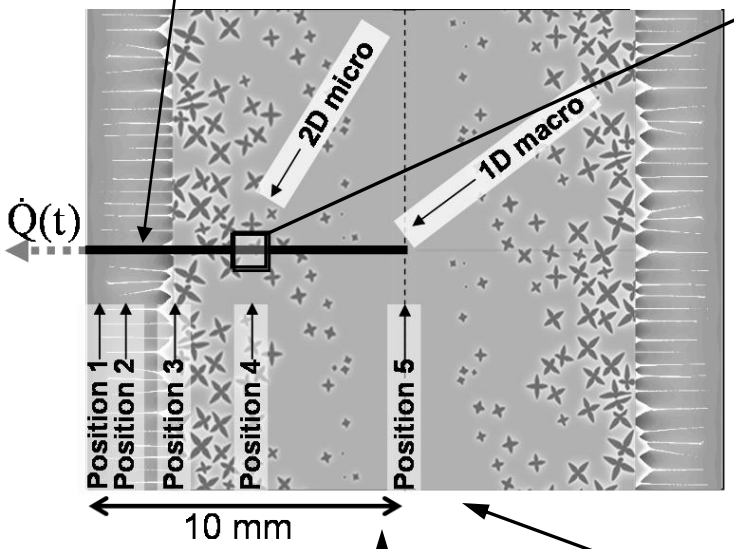


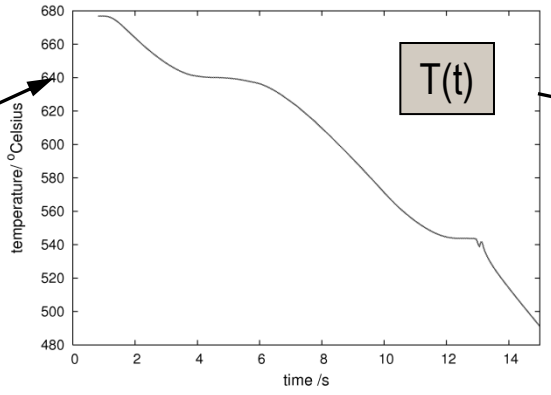
temperature equation for 1D solver:

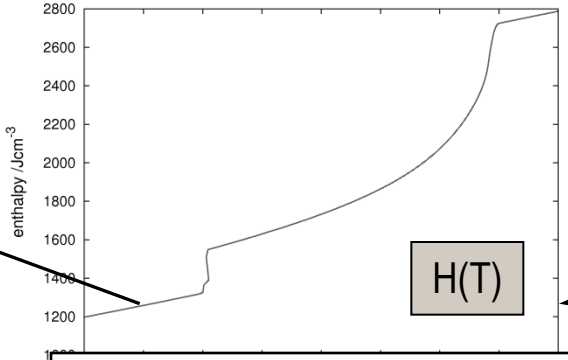
$$dT^i = \frac{1}{\bar{C}_p^i}\left(\lambda^i\frac{d^2T}{dx^2}dt - dL^i\right), \quad dL^i = dH^i - \bar{c}_p^i{}' dT^{i\prime}$$

Linking to the Process: A Virtual Solidification Experiment for Al-3at%Cu Plate Casting

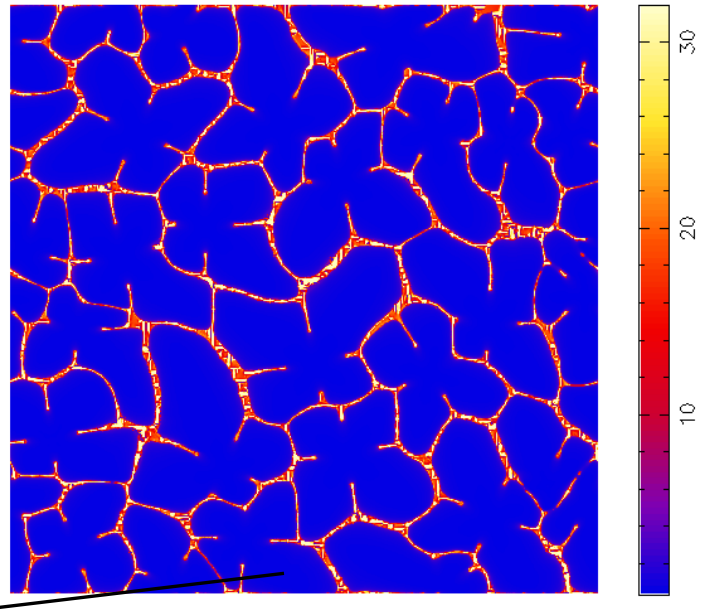
macroscopic temperature field
(1D approximation)







microstructure
simulation



H(T)

Scheil approximation

thermodynamic data

what happens if wee feed back H(T) to macro-scale?
→ “homoenthalpic” approximation!

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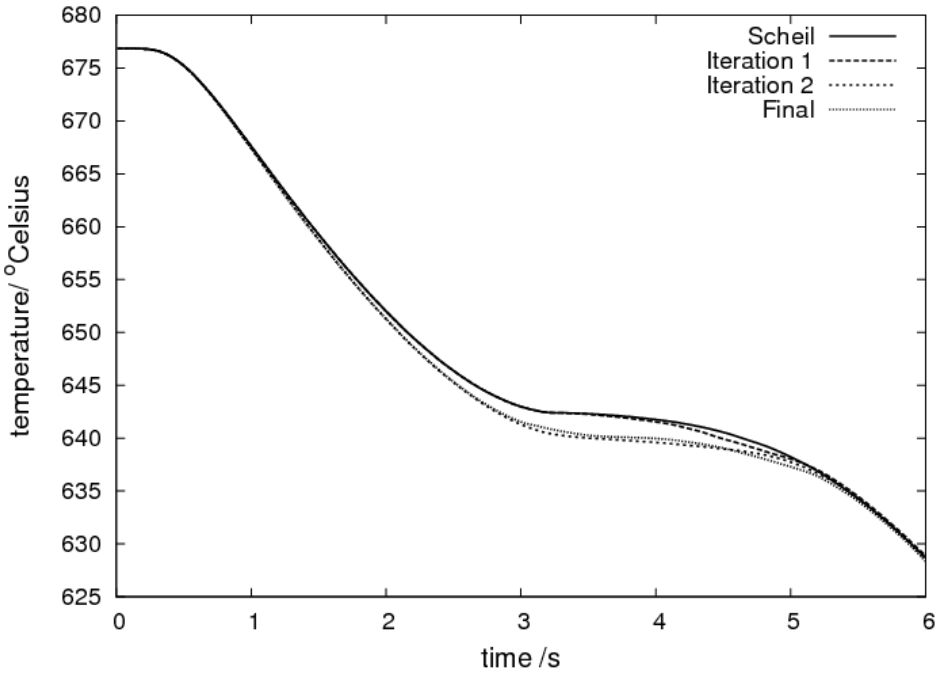
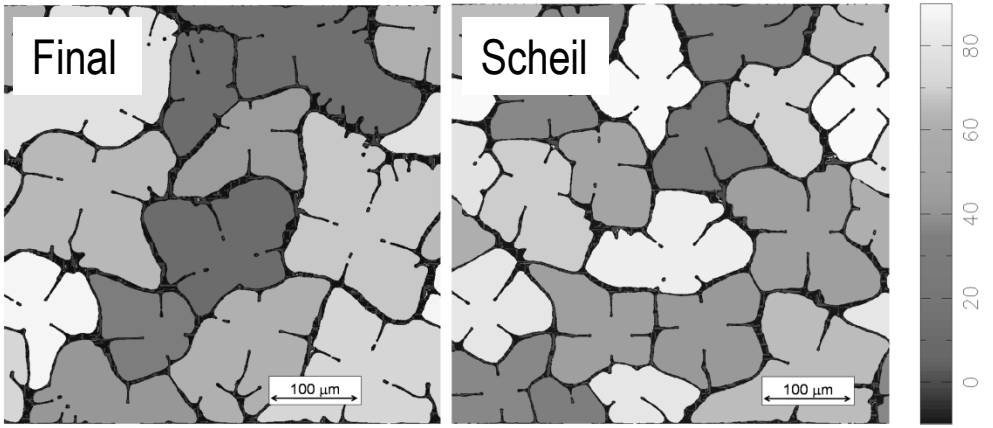
Linking to the Process: Homoenthalpic Approach

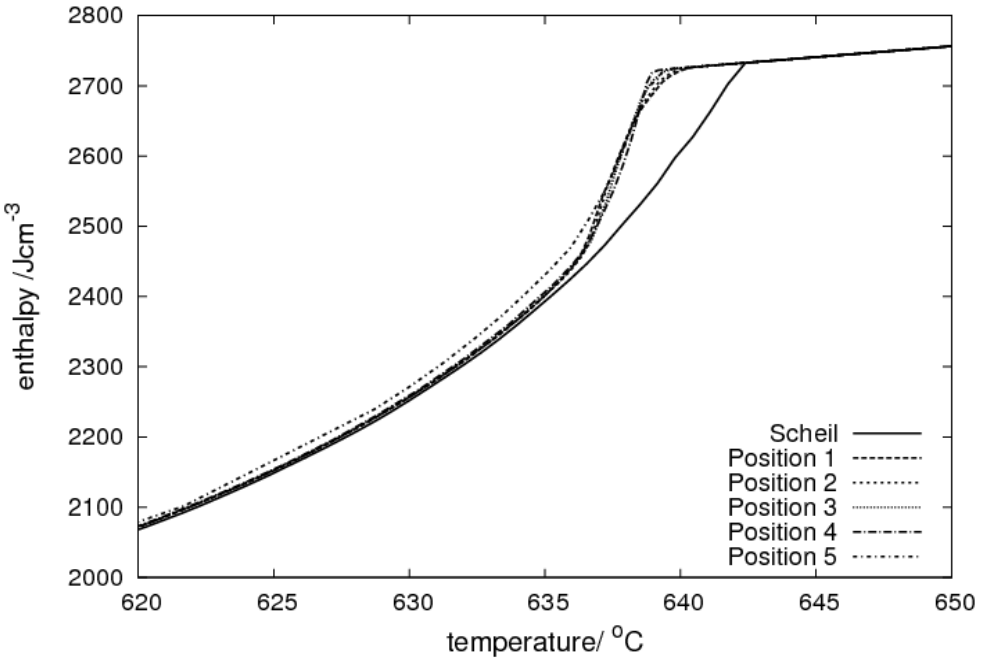


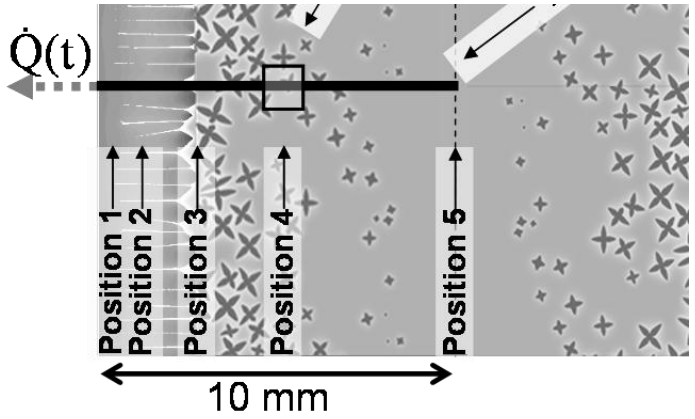
- converging rapidly, leading to a self-consistent solution
- differences are small, but in critical temperature range

➡ Strong effect on grain size!



Linking to the Process: Homoenthalpic Approach





- after iteration H(T) is very similar for different positions in the virtual casting!
- Homoenthalpic approximation (assumption of a global H(T) relation) is reasonable in this case!

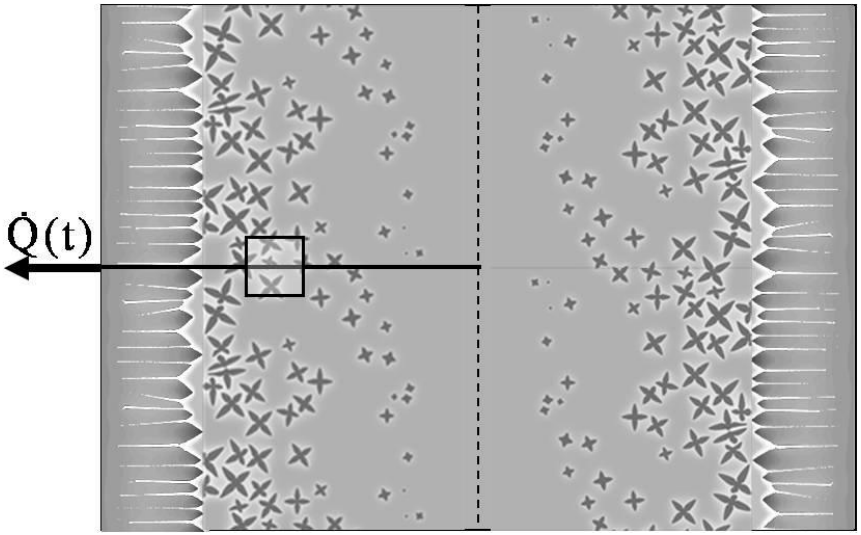
Homoenthalpic Approach allows for an iterative solution of the general micro-macro problem!

Example 8:

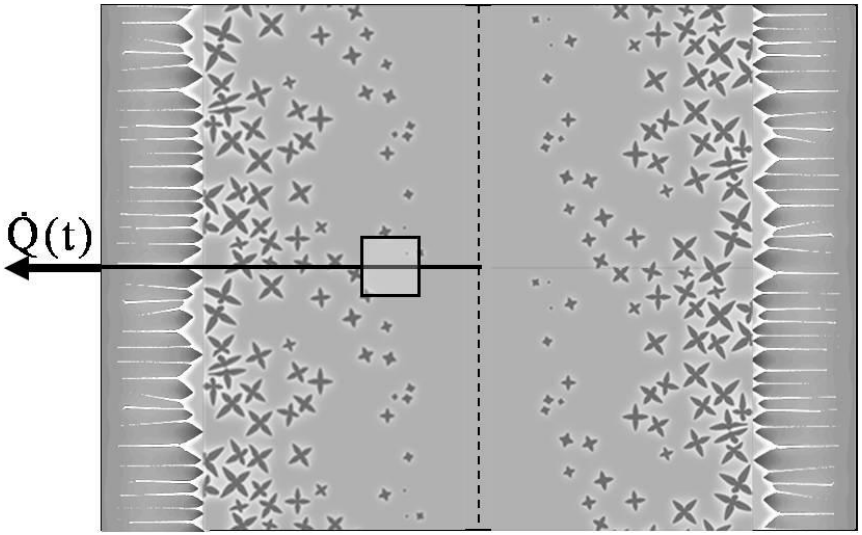
Equiaxed Solidification of IN738

Equiaxed Solidification of IN738: Comparison of 2 Positions of Microdomain

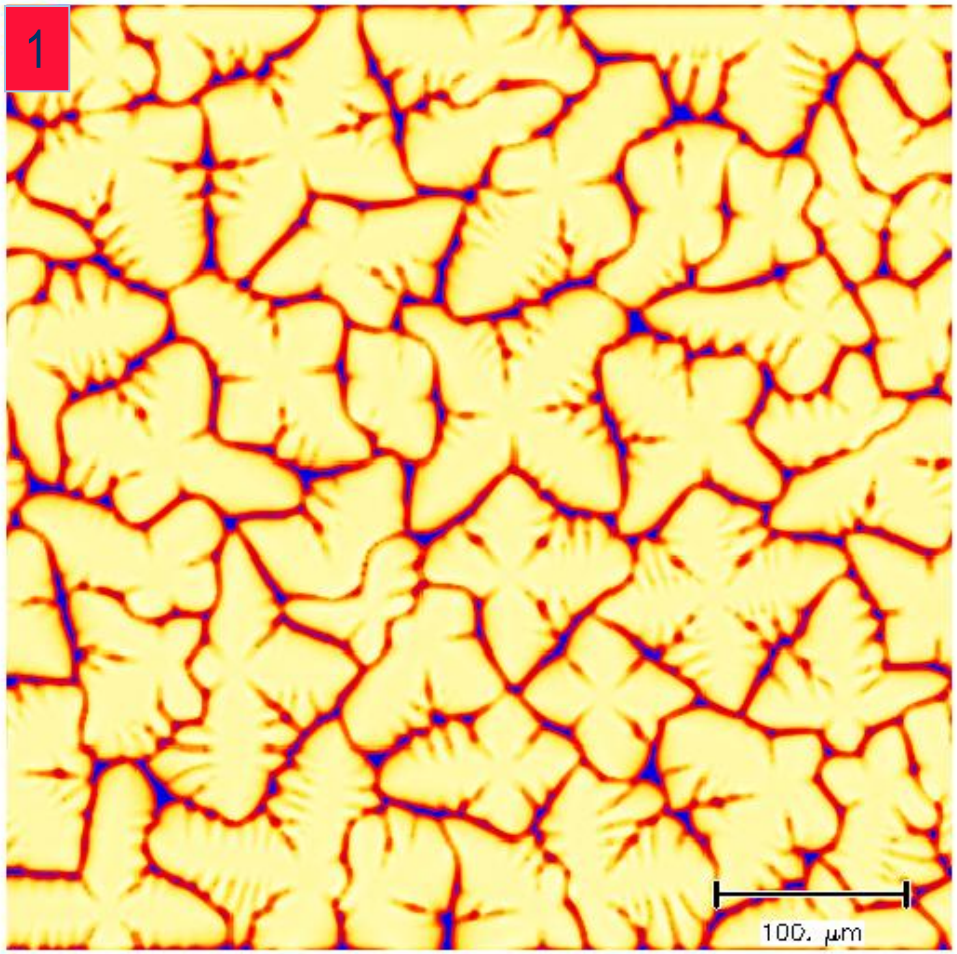
Position 1

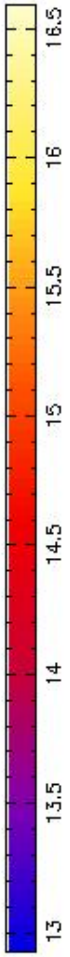


Position 2

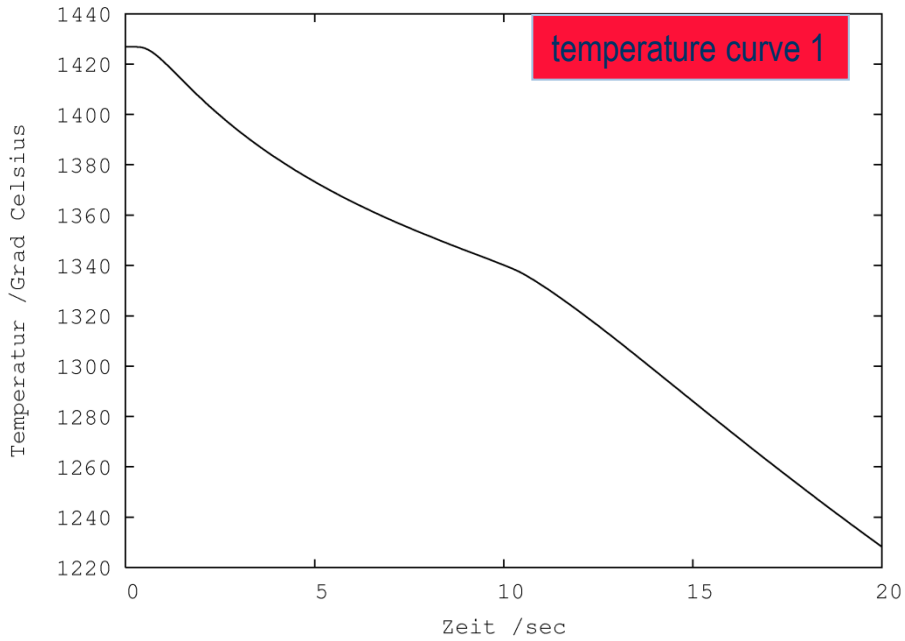


Equiaxed Solidification of IN738

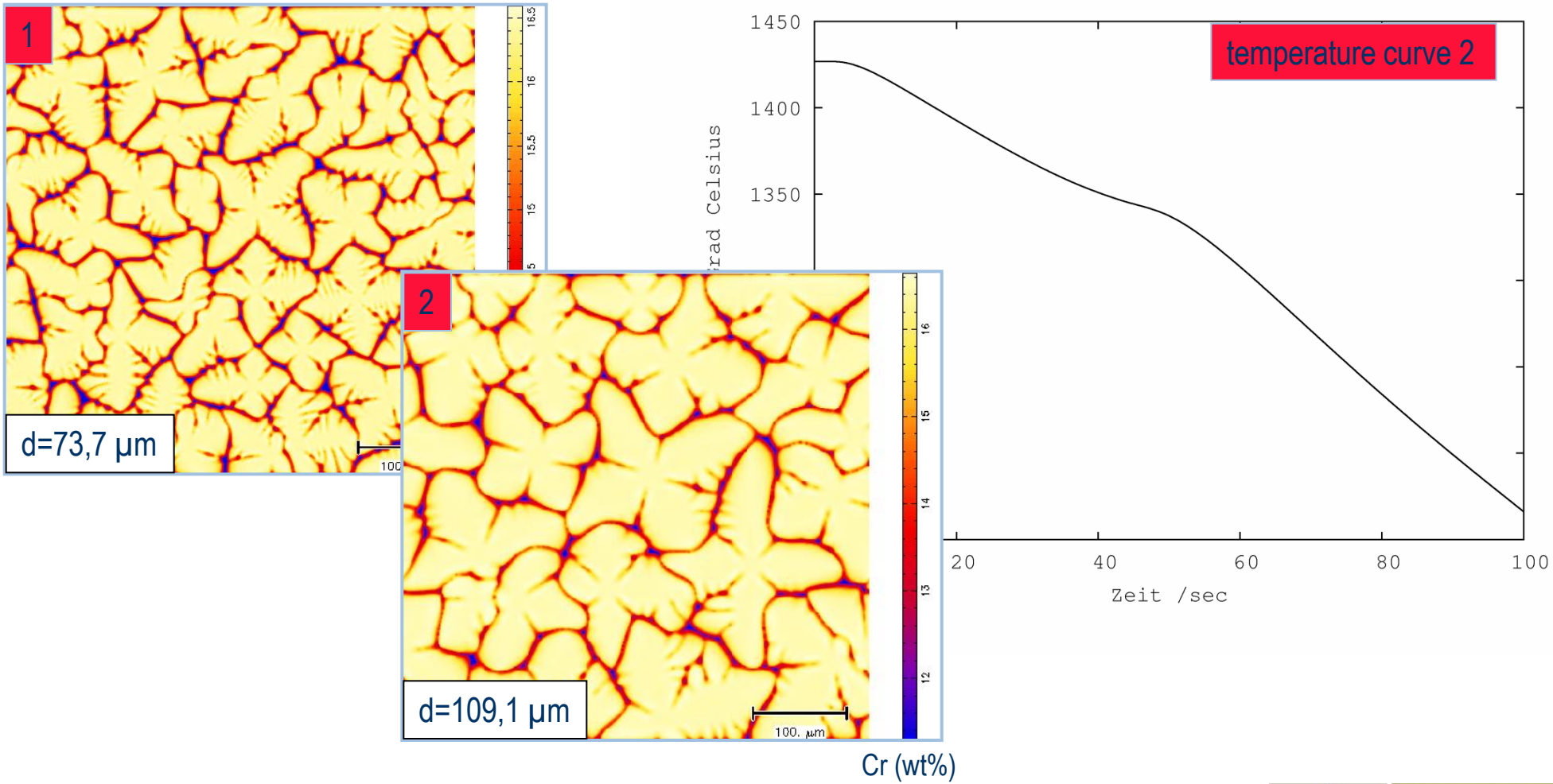




Cr (wt%)

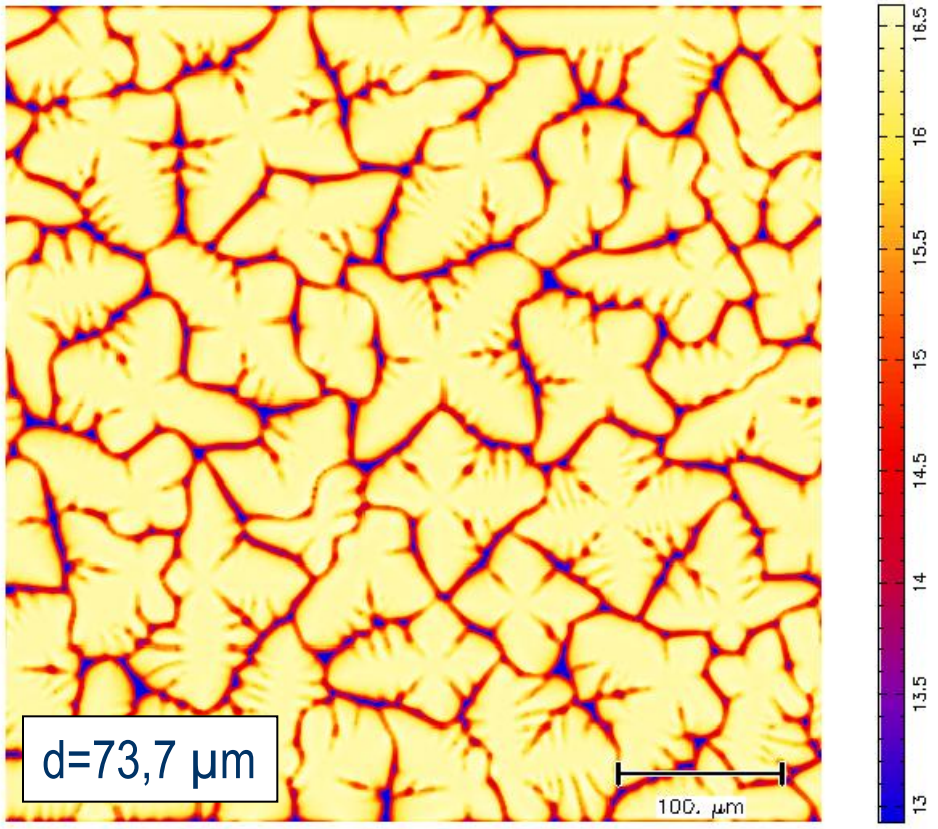


Equiaxed Solidification of IN738: Different Cooling Conditions

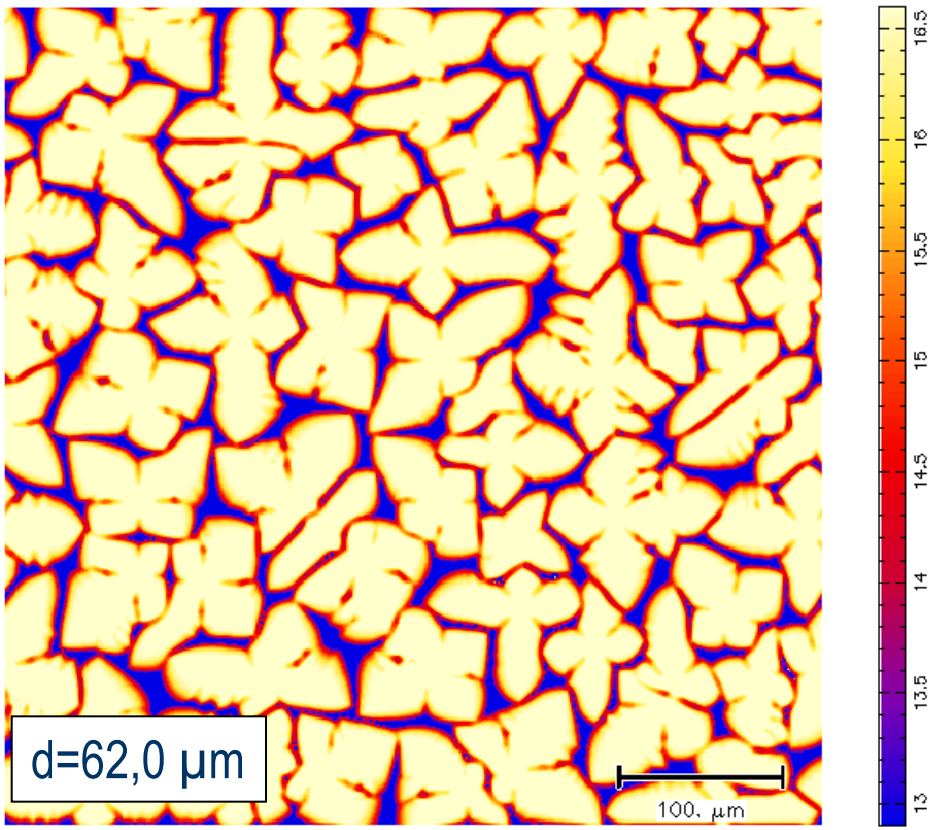


Equiaxed Solidification of IN738: Different Composition

IN738



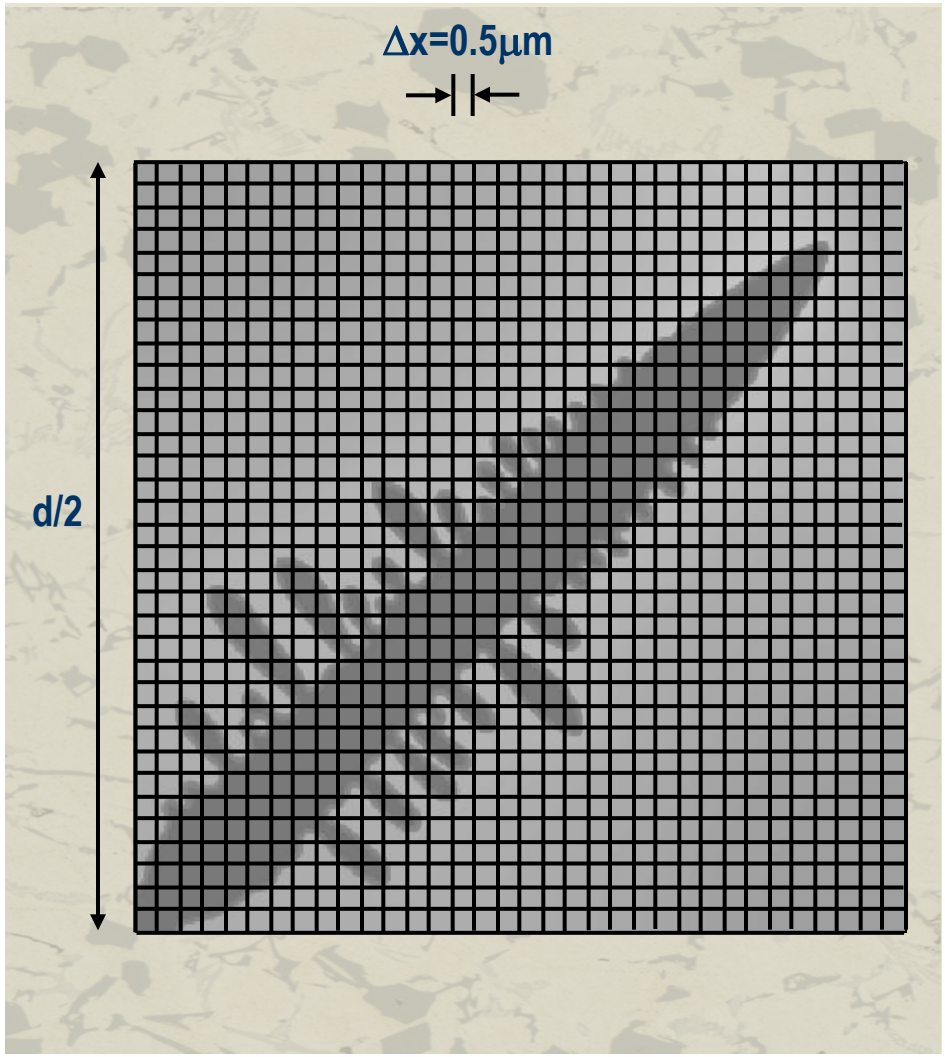
IN738 + 2% Nb



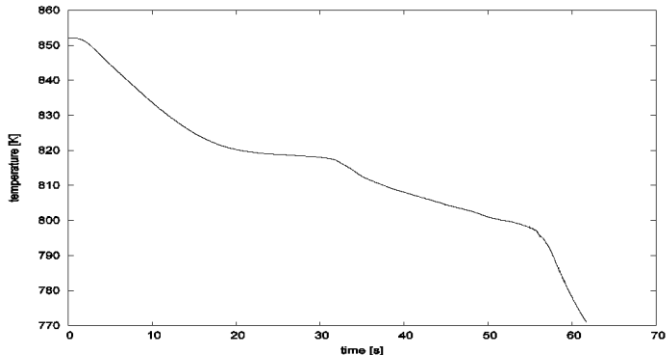
Example 9:

Piston Alloy KS1295

Piston Alloy KS1295: Simulation Setup



- include elements Al Si Cu Mg Ni Fe Mn Zn
- include all phases which may appear during solidification
- unit cell model for ¼ grain
- FD grid with 400 x 400 cells and 0.5 µm resolution
- realistic temperature field from external 1D simulation using the Homoenthalpic Approximation



- coupling to thermodynamic database TTAL5
- coupling to diffusion database MOBAL1

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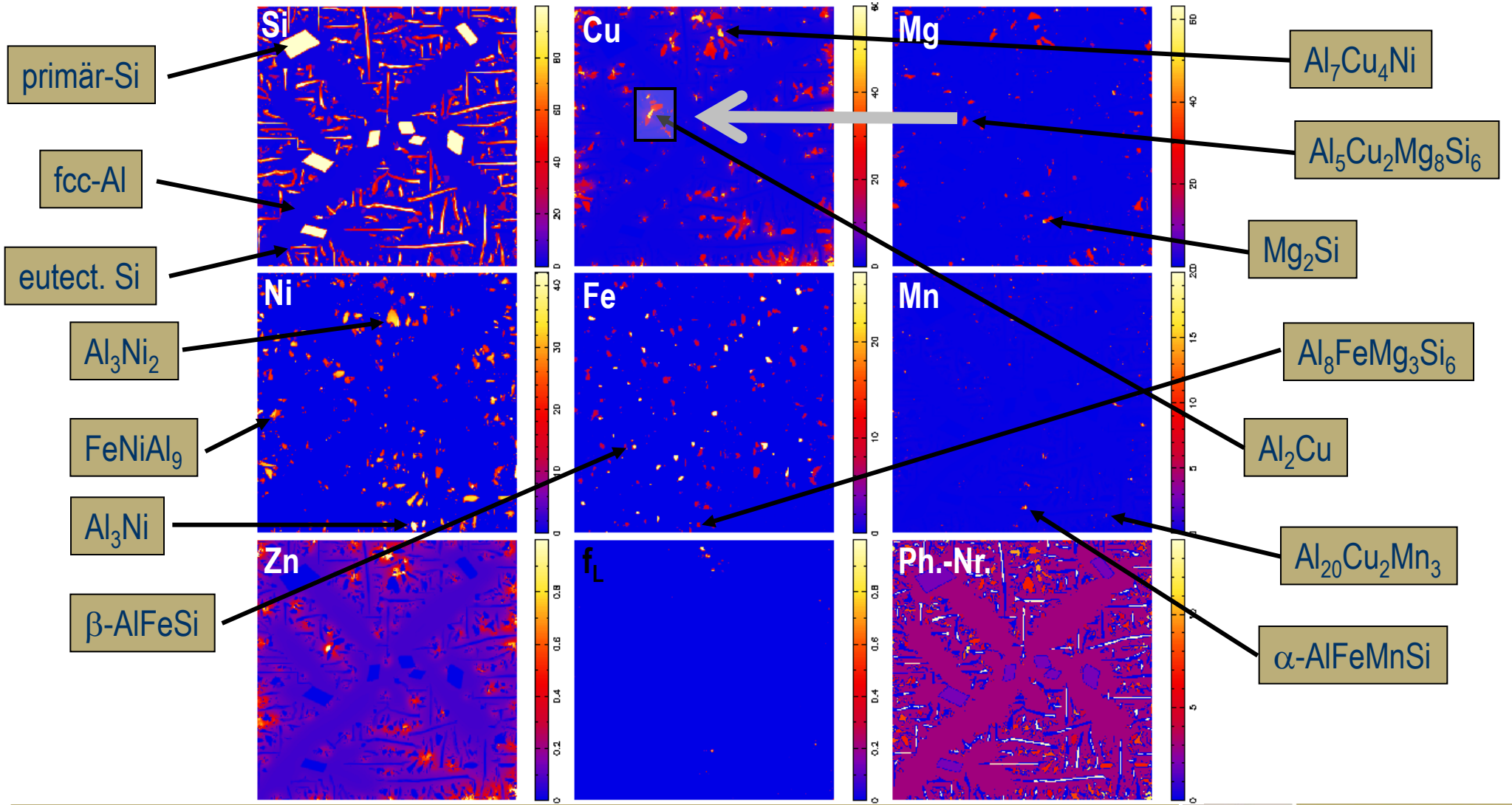
Piston Alloy KS1295: Segregation and Intermetallic Phases



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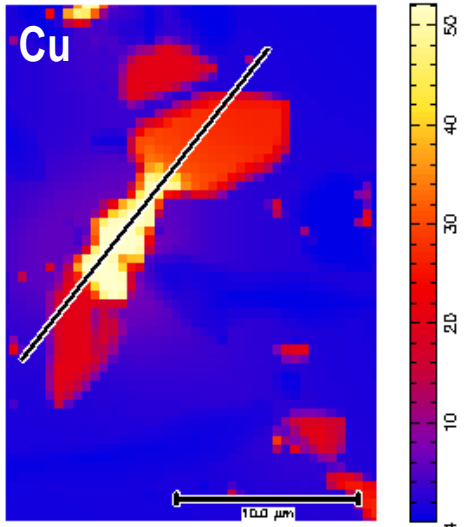
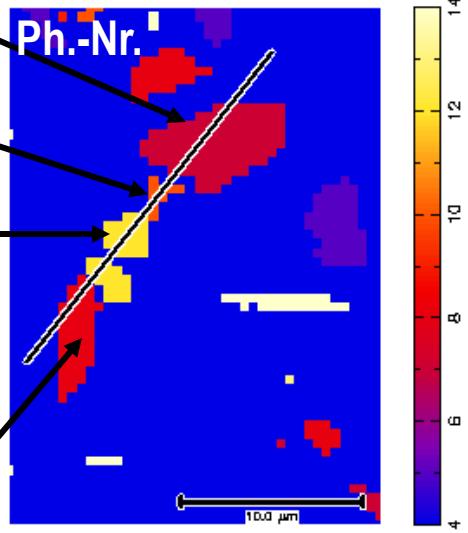
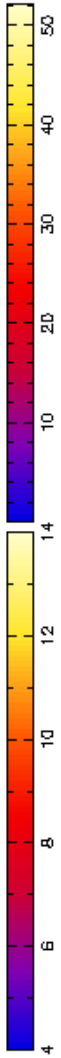
Piston Alloy KS1295: Simulation Details





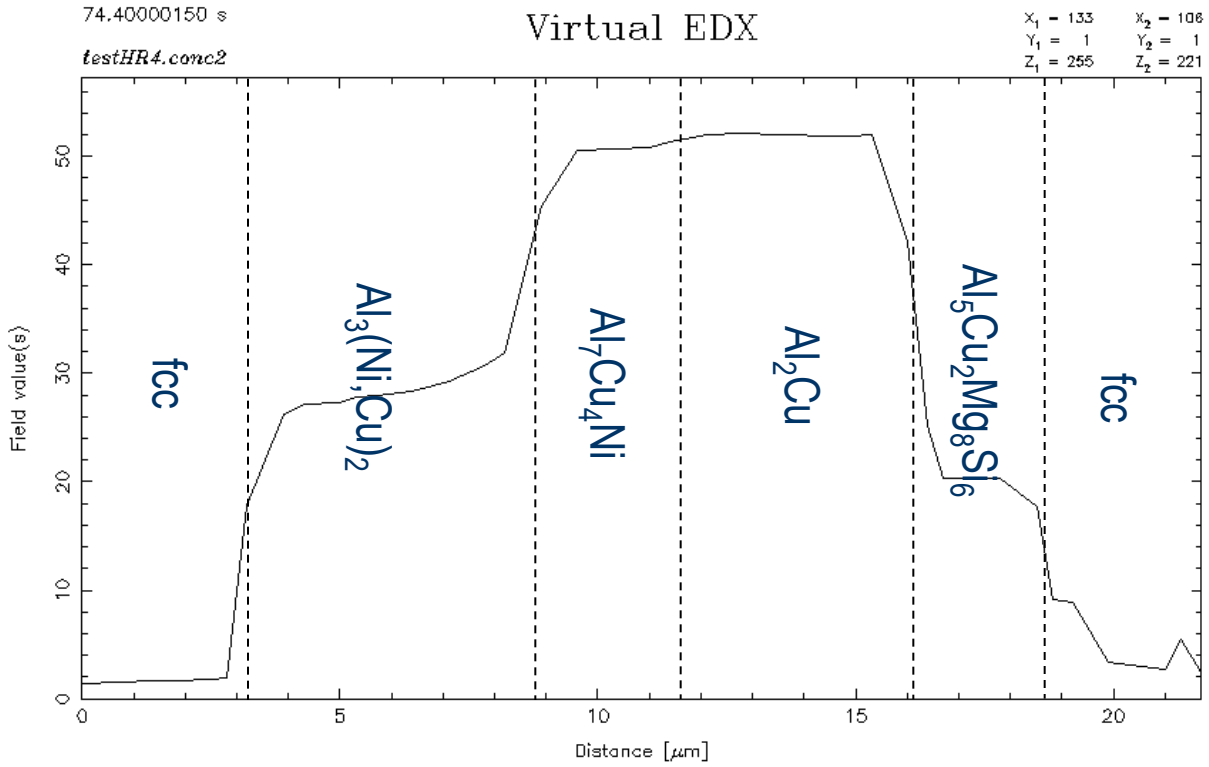


Al_3Ni_2

Al_7Cu_4Ni

Al_2Cu

$Al_5Cu_2Mg_8Si_6$



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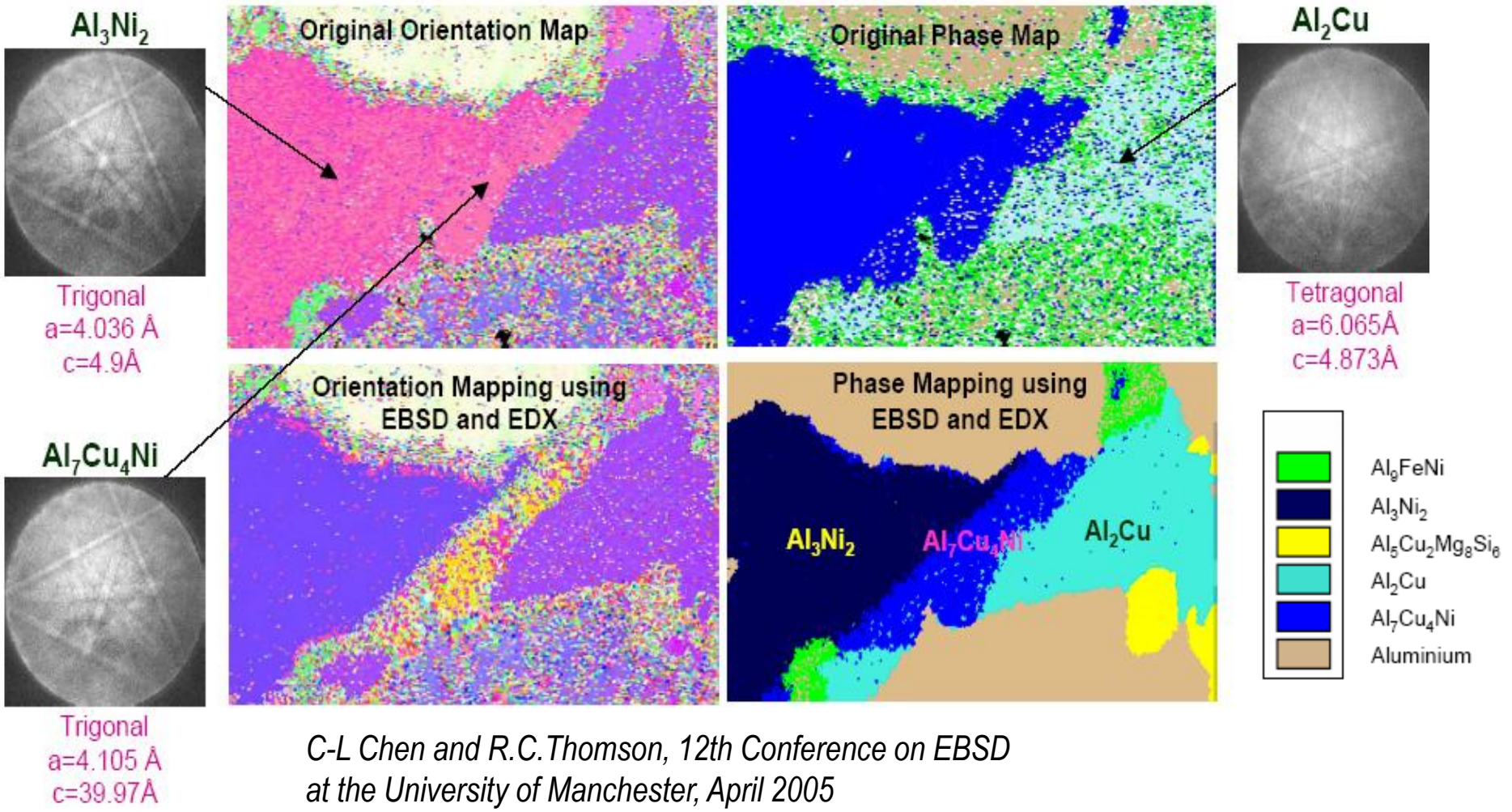
Phase Identification using EDX and EBSD (piston alloy similar to KS1295)



C-L Chen and R.C.Thomson, 12th Conference on EBSD at the University of Manchester, April 2005

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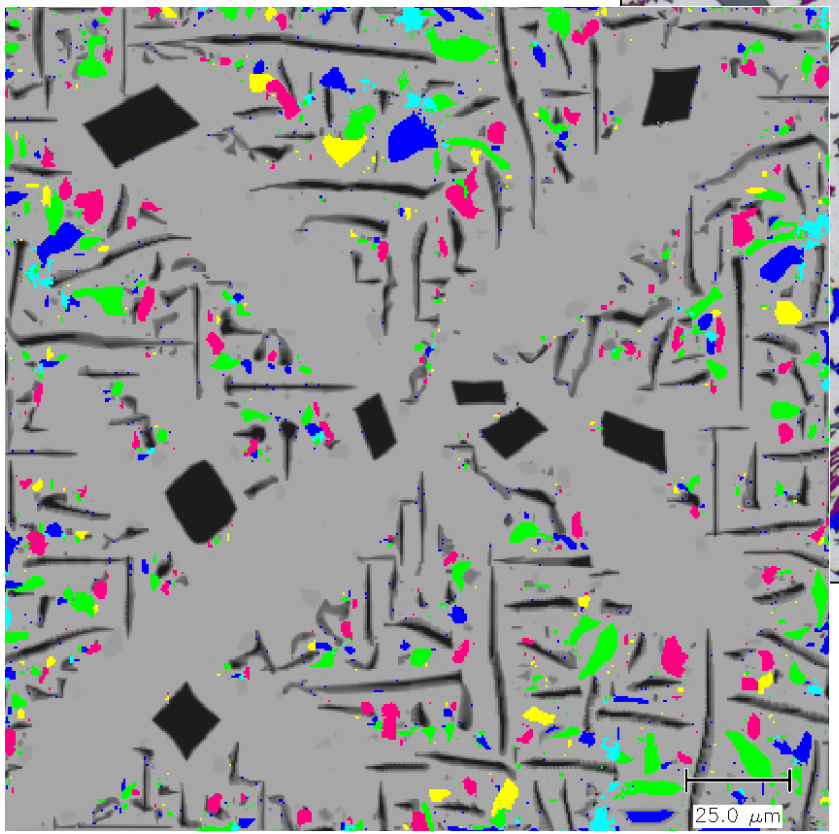
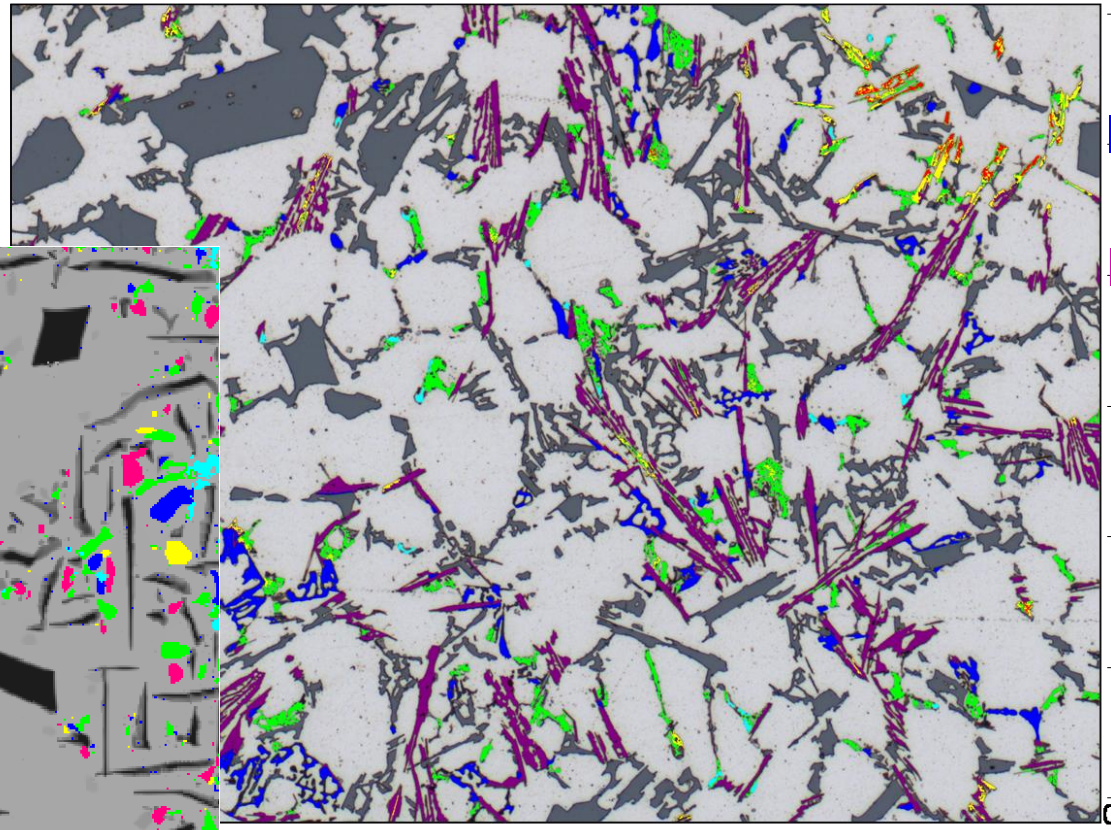
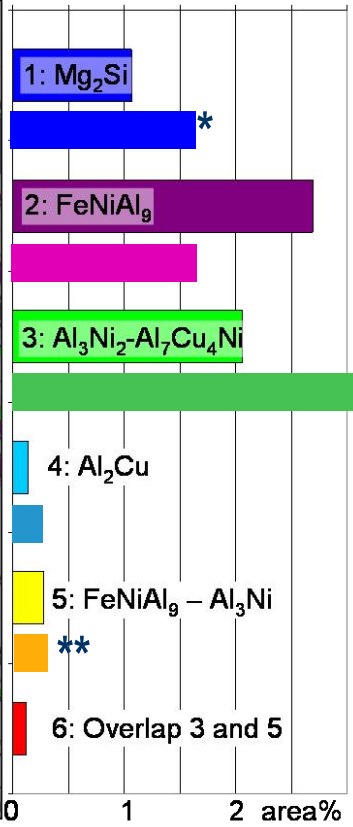
Example1: Alloy KS1295 (Al-Si-Fe-Ni-Cu-Mg-Zn), Comparison to Quantitative Metallography







- databases: TTAL5, MOBAL1
- collaboration with *Kolbenschmidt/Germany* and *University of Manchester*

* **$Mg_2Si + Al_5Cu_2Mg_8Si$**
** **Al_3Ni**

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5. **Conclusion**

Conclusion

- For PF microstructure simulation in complex technical applications a “pragmatic” phase-field approach has to be used
- One needs a proper multiphase-field model which can be applied at various length scales
- Coupling to thermodynamic databases and mobility data is essential for simulation of multicomponent alloys
- Pragmatic approximations have to be found to appropriately couple the PF model to the process conditions
- MICRESS® is a commercial software package developed in our research group at ACCESS/Germany which can be applied for research, education and industrial applications

Thank you for

your attention!