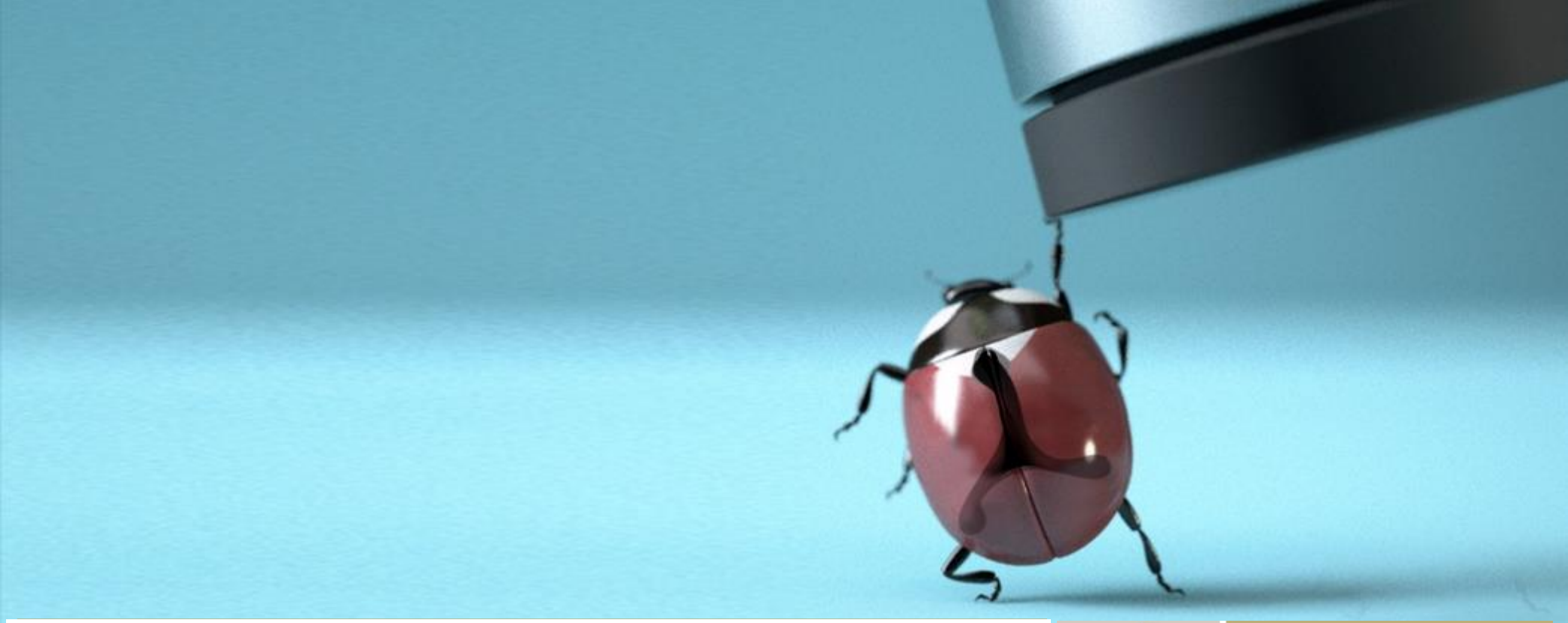


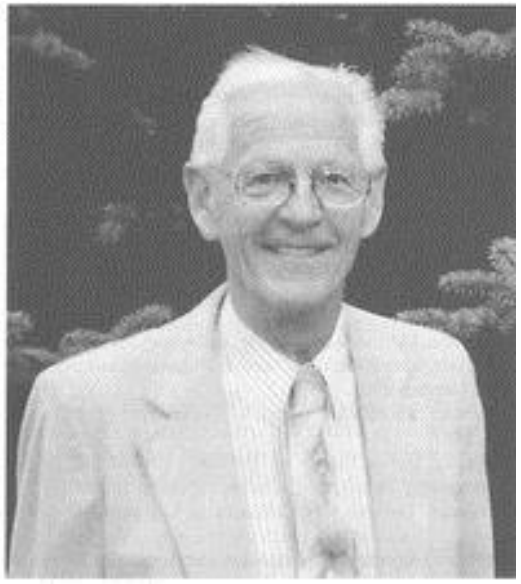
From Massalski to MICRESS and beyond: An introduction to MICRESS and current trends in Integrated Computational Materials Engineering “ICME”

Dr. rer.nat. Georg J. Schmitz

Version August 2014

Thaddeus B. Massalski

First Edition 1986



Born in Warschau 1926

Ph.D., University of Birmingham, 1954

Carnegie Mellon University since 1959

Stability of alloy phases, imperfections in crystals, phase transformations and amorphous structures.

about 1980:

first networks / Internet

about 1960

1973: my first calculator (DM 300,--) …150 €

Thermodynamics AND Computer

„I disliked computers. Thus I started studying metallurgy, because I thought this subject would be too complicated to be ever put on a computer……“

Bo Sundman ,
one of the creators of ThermoCalc

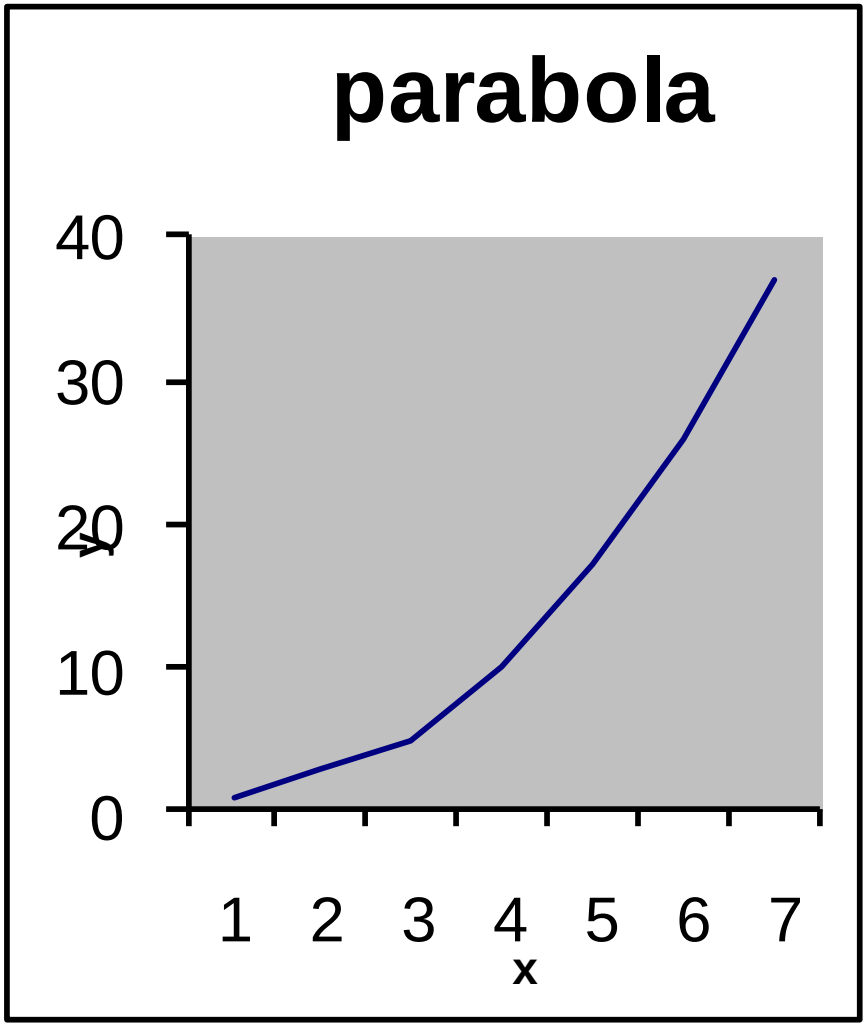
What are thermodynamic databases ?

thermodynamic databases are NOT (!!) just

collections of experimental data in an Excel sheet !!

Thermodynamic databases are based on physical models allowing extrapolations into „unknown areas“

A (thermodynamic) database in our understanding means a collection of polynomials describing the Gibbs energy of individual phases of a system as a function of temperature, (pressure) and composition.



example:

$$y-y_0 = a(x-x_0)^2$$

here: $y_0=1$ $a=1$ $x_0=0$

Example: binary alloy with elements A and B

$$G_m - H_m^{SER} = a + bT + cT\ln(T) + \sum d_i T^i$$

$$G_m = G_m^0 + \Delta G_m^{ideal} + \Delta G_m^{xs}$$

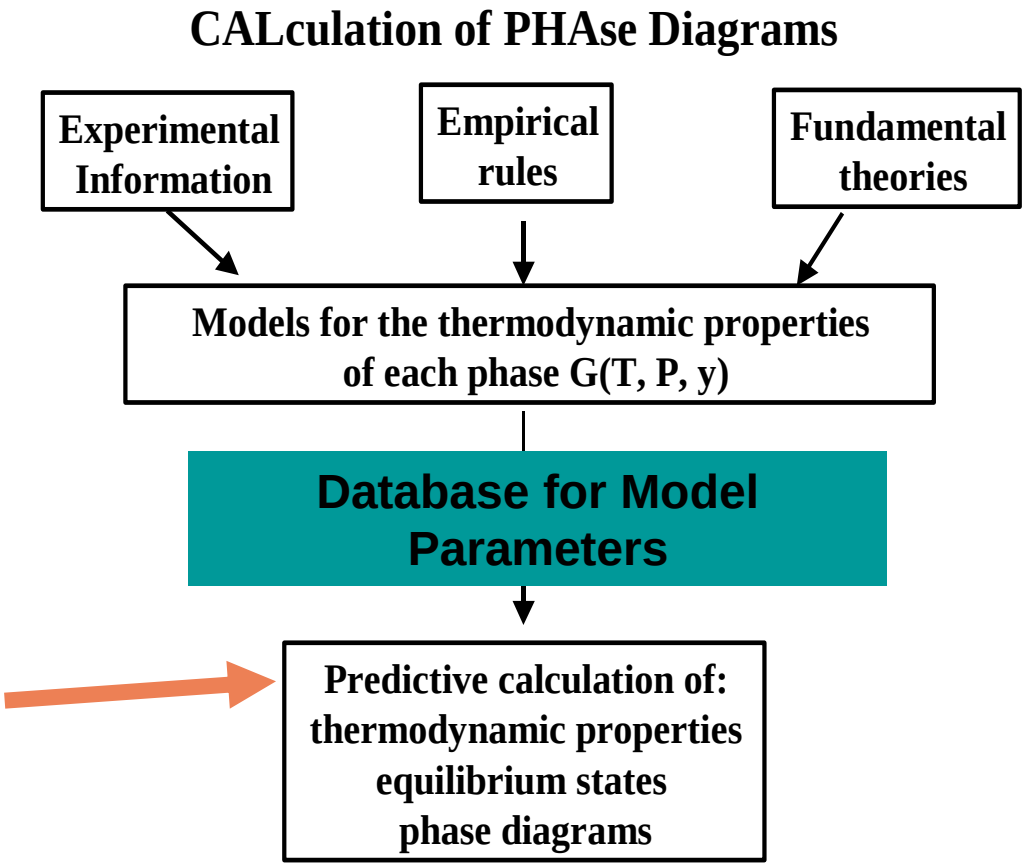
$$G_m^0 = x_A G_A^o + x_B G_B^o$$

$$\Delta G_m^{ideal} = RT\left(x_A \ln x_A + x_B \ln x_B\right)$$

$$\Delta G_m^{xs} = x_A x_B \sum_{k=0} {}^kL_{A,B}(x_A - x_B)^k$$

$$= x_A x_B \left({}^0L_{A,B} + {}^1L_{A,B}(x_A - x_B) + {}^2L_{A,B}(x_A - x_B)^2 \ldots.\right)$$

The CALPHAD method

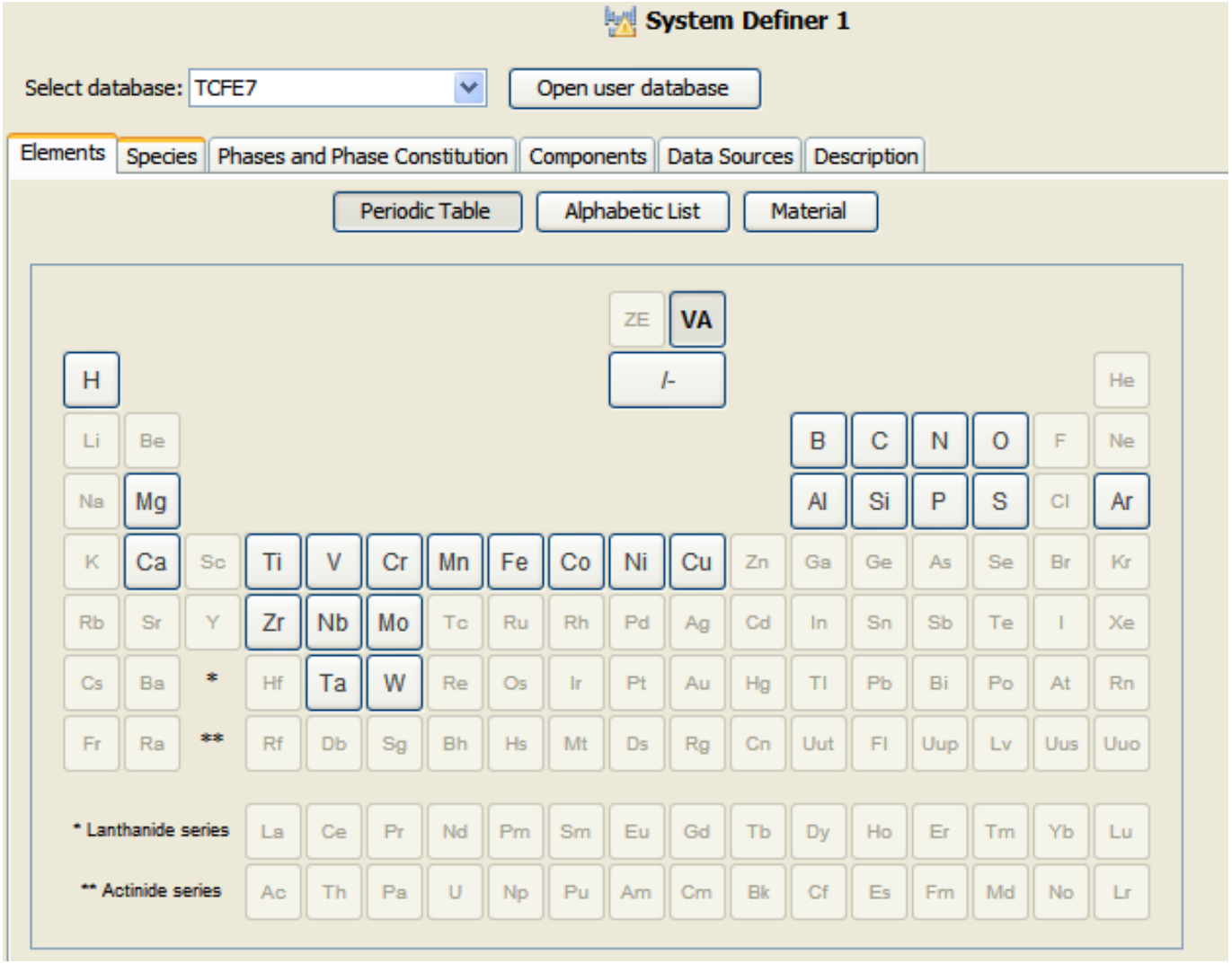


- www.calphad.org
- 1969 Formation of CALPHAD.
- 1971 Sub-lattice model for 2 comp. (Hillert and Steffansson, KTH).
- 1977 Development of Thermo-Calc starts

Examples of available databases

- Steels and Fe-alloys
- Nickel-base superalloys
- Aluminium/Titanium/Magnesium-base alloys
- Gases, pure inorganic/organic substances, & general alloys
- Slag, metallic liquids, and molten salts
- Ceramic systems, and hard materials
- Semiconductors, and solder alloys
- Nobel metal alloys
- Materials processing, process metallurgical & environmental aspects
- Aqueous solutions, materials corrosion & hydrometallurgical systems
- Minerals, and geochemical/environmental processes
- Nuclear materials, and nuclear fuel/waste processing

Elements in the steel database (TCFe7)



Phases in TCFe7

- A1_KAPPA
- AF
- AL2S3
- AL2TIO5
- AL4C3
- ALN
- ALPHA_SPINEL
- ANDALUSITE
- ANORTHITE
- B2M
- B2_BCC
- B2_VACANCY
- B3SI
- B4C
- BCC_A2
- BETA_RHOMBO_B
- BM
- BN_HP4
- C1A1
- C1A2
- C1A6
- C1A8M2
- C2A14M2
- C2F
- C3A1
- C3A2M1
- C4WF4
- C4WF8
- CA1CR2O4_A
- CA1CR2O4_B
- CA2SIO4_ALPHA
- CA2SIO4_ALPHA_PRIME
- CAMN2O4
- CAMNO3
- CEMENTITE
- CF
- CF2
- CHI_A12
- CLINO_PYROXENE
- CORDIERITE
- CORUNDUM_M2O3
- CR2B_ORTH
- CR3SI
- CRB2
- CRISTOBALITE
- CU3P
- CW3F
- CWF
- DIAMOND_FCC_A4
- DICTRA_FCC_A1
- DIGENITE
- FCC_A1
- FC_ORTHORHOMBIC
- FE2S3O12
- FE2SI
- FE4NB2O9
- FE4N_LP1
- FE8SI2C
- FECN_CHI
- FEP
- FESO4
- FLUORITE_C1
- GAS
- GRAPHITE
- G_PHASE
- HALITE
- HATRURITE
- HCP_A3
- HIGH_SIGMA
- KAPPA
- KSI_CARBIDE
- KYANITE
- L12_FCC
- LARNITE
- LAVES_PHASE_C14
- LIQUID
- LOWCLINO_PYROXENE
- M12C
- M23C6
- M2B_TETR
- M2P
- M3B2
- M3C2
- M3P
- M3SI
- M5C2
- M5SI3
- M6C
- M7C3
- MB_B33
- MC_ETA
- MC_SHP
- MELILITE
- MERWINITE
- MG2NI
- MG2SI
- MGC2
- MN1O2
- MN2O3
- MN6N4
- MN6N5
- MNS
- MO2B5
- MSI
- MULLITE
- MU_PHASE
- NBNI3
- NBO
- NI3S2
- NI3TI
- NI6MNO8_TYPE
- NIMNO3
- NITI2
- OLIVINE
- ORTHO_PYROXENE
- PI
- PROTO_PYROXENE
- PSEUDO_WOLLASTONITE
- PYRRHOTITE
- P_PHASE
- QUARTZ
- RANKINITE
- RED_P
- RHODONITE
- RUTILE_MO2
- R_PHASE
- S2ZR1
- SAPPHIRINE
- SI3N4
- SIC
- SIGMA
- SILLIMANITE
- SILLIMANITE
- SIS2
- SPINEL
- TAN_EPS
- TI2N
- TI3O2
- TI4C2S2
- TIO
- TIO_ALPHA
- TRIDYMITE
- WHITE_P
- WOLLASTONITE
- ZR2S3
- ZRO2_MONO
- ZRO2_TETR
- Z_PHASE

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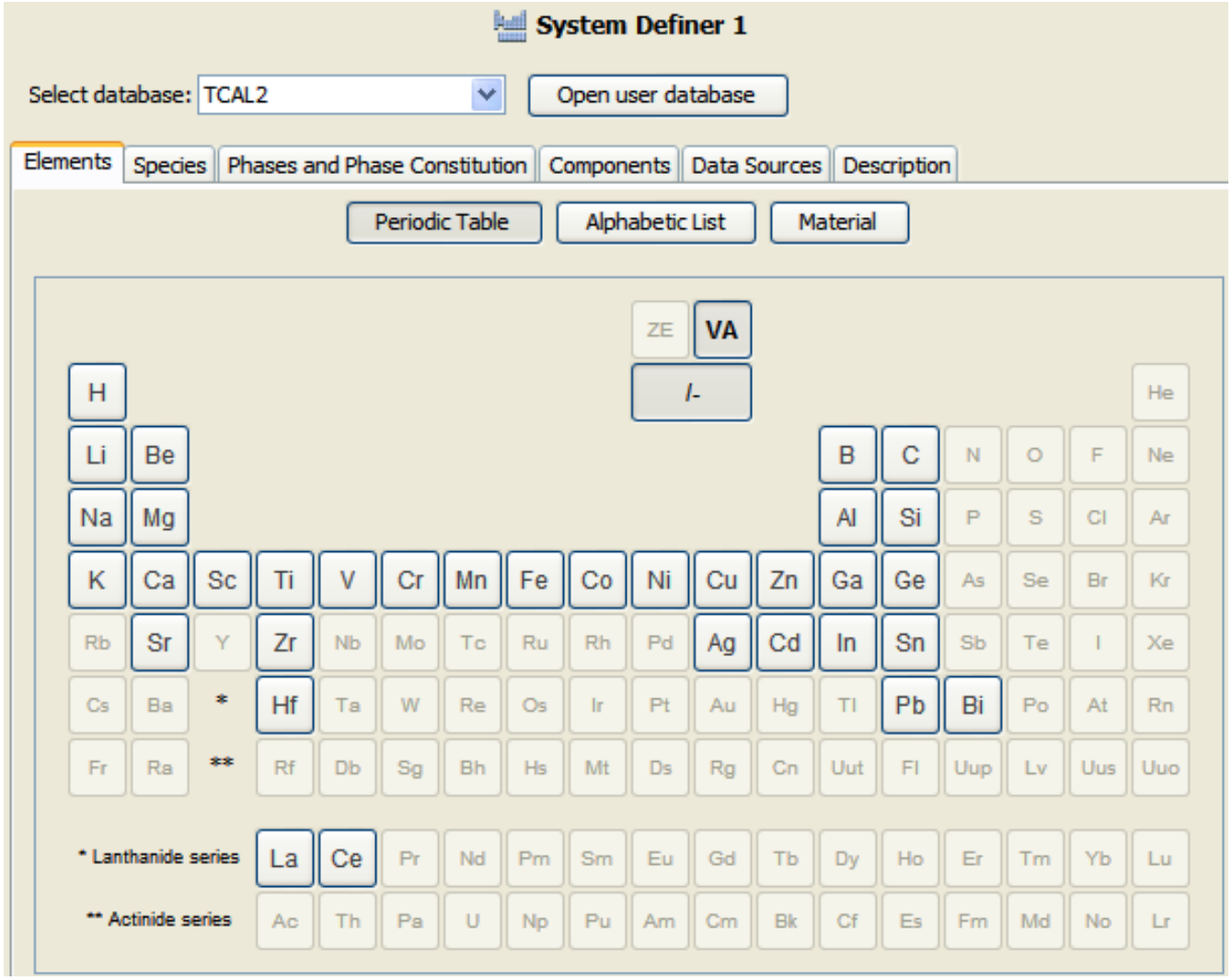
access

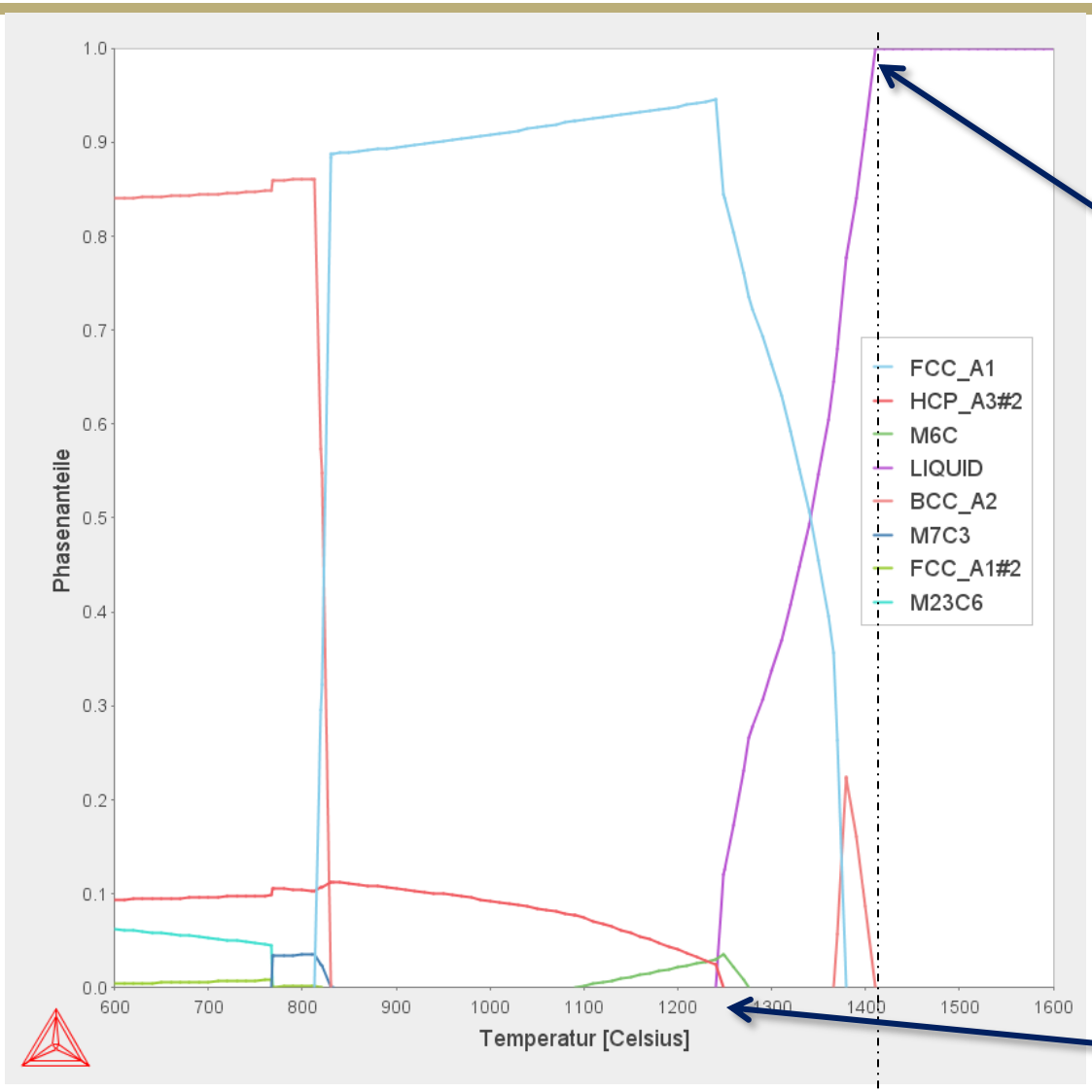
Elements in the Aluminum database TCAl2



More than 190 phases in COST Al-alloys database

LIQUID:L
ALB2
ALB12_ALPHA
ALB12_BETA
AL4C3
AL4SIC4
AL8SIC7
ALCE_AMORPHOUS
ALCR2
AL4CR
AL8CR5_H
AL8CR5_L
AL9CR4_H
AL9CR4_L
AL11CR2
AL13CR2
ALCU_DELTA
ALCU_EPSILON
ALCU_ETA
ALCU_THETA
ALCU_PRIME
ALCU_ZETA
ALCULI_TB
ALCULI_R
ALCULI_T1
ALCULI_T2
ALCUZN_T
AL13FE4
AL2FE
AL5FE2
ALFESI_ALPHA
ALFESI_BETA
ALFESI_GAMMA
ALFESI_DELTA
ALFESI_TAU1
ALFESI_TAU3
ALLI
AL2LI3
AL4LI9
AL12MG17
ALLIMG_TAU
ALMG_BETA
ALMG_EPS
ALMG_GAMMA
ALMGMN_T
AL11MN4
AL12MN
AL4MN
AL6MN
AL8MN5_D810
ALMNSI_ALPHA
ALMNSI_BETA
ALMNSI_DELTA
AL12MO
AL4MO
AL5MO
AL63MO37
AL8MO3
ALMO
ALN
ALND_AMORPHOUS
ALTI
ALM_D019
AL2TI
AL3M_D022
AL11TI5
AL7V
AL8V5
AL10V
AL23V4
AL12W
AL2W
AL4W
AL5W
AL7W3
AL77W23
AL3ZR
AL2ZR
BETA_RHOMBO_B
B4C
B_NSI
BN_HP4
B3SI
B6SI
BTI
B4TI3
B2TI
BM
B4M3
B2M
BCC_A2
BCC_B2
CBCC_A12
BCT_A5
CSI
CR3MN5
CR3SI_A15
CUB_A15
CR5SI3
CRSI
CRSI2
CRZN13
CRZN17
CUMGSI_SIGMA
CUMGSI_TAU

First benefits….



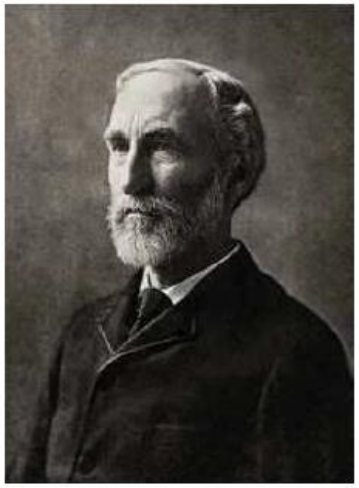
Fe-4Cr-8Mo-2V-0.3Mn-0.3Si-1C

T_{liq} ~ 1410°C

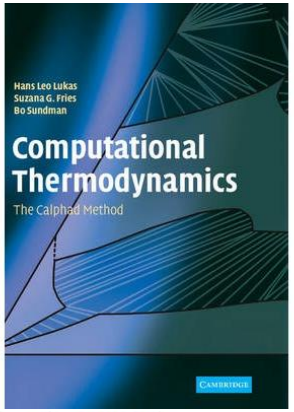
T_{sol}~ 1240 °C

more benefits: calculation of thermodynamic properties

Gibbs energy	G	$=$	$G(T, p, N_i)$
entropy	S	$=$	$-\left(\frac{\partial G_m}{\partial T}\right)_{p,N_i}$
enthalpy	H	$=$	$G + TS = G - T\left(\frac{\partial G}{\partial T}\right)_{p,N_i}$
volume	V	$=$	$\left(\frac{\partial G}{\partial p}\right)_{T,N_i}$
Chemical potential of component i	μ_i	$=$	$\left(\frac{\partial G}{\partial N_i}\right)_{T,N_{j\neq i}}$
heat capacity	C_p	$=$	$-T\left(\frac{\partial^2 G}{\partial T^2}\right)_{p,N_i}$
thermal expansion	α	$=$	$\frac{1}{V}\left(\frac{\partial^2 G}{\partial p \partial T}\right)_{N_i}$
isothermal compressibility	κ	$=$	$-\frac{1}{V}\left(\frac{\partial^2 G}{\partial p^2}\right)_{T,N_i}$
bulk modulus	B	$=$	$\frac{1}{\kappa}$



Josiah Willard Gibbs

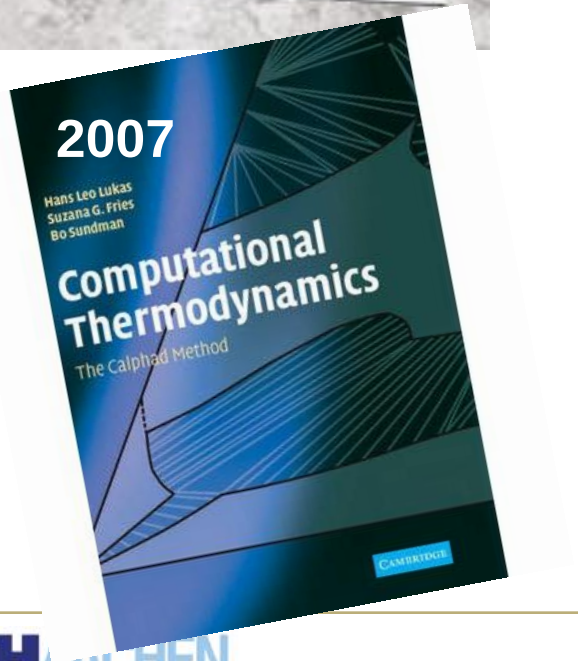


from Hans Lukas, Suzana G. Fries, Bo Sundman
Computational Thermodynamics, The Calphad Method, 2007

Computational Thermodynamics (phase equilibria)

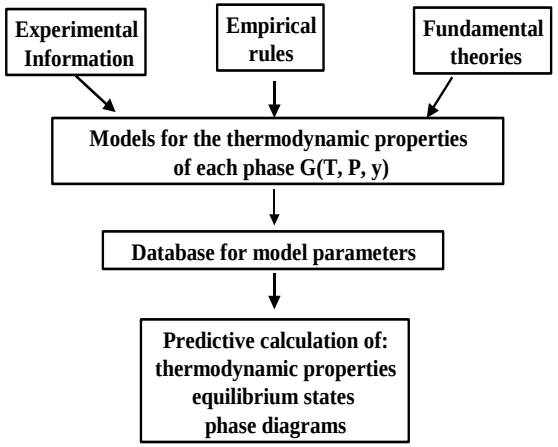
„I disliked computers. Thus I started studying metallurgy, because I thought this subject would be too complicated to be ever put on a computer……"

Bo Sundman, one of the creators of Thermo-Calc



The CALPHAD method

CALculation of PHAse Diagrams



www.calphad.org

1969 Formation of CALPHAD.

1971 Sub-lattice model for 2 comp. (Hillert and Steffansson, KTH).

1977 Development of Thermo-Calc starts

Intermediate summary 1

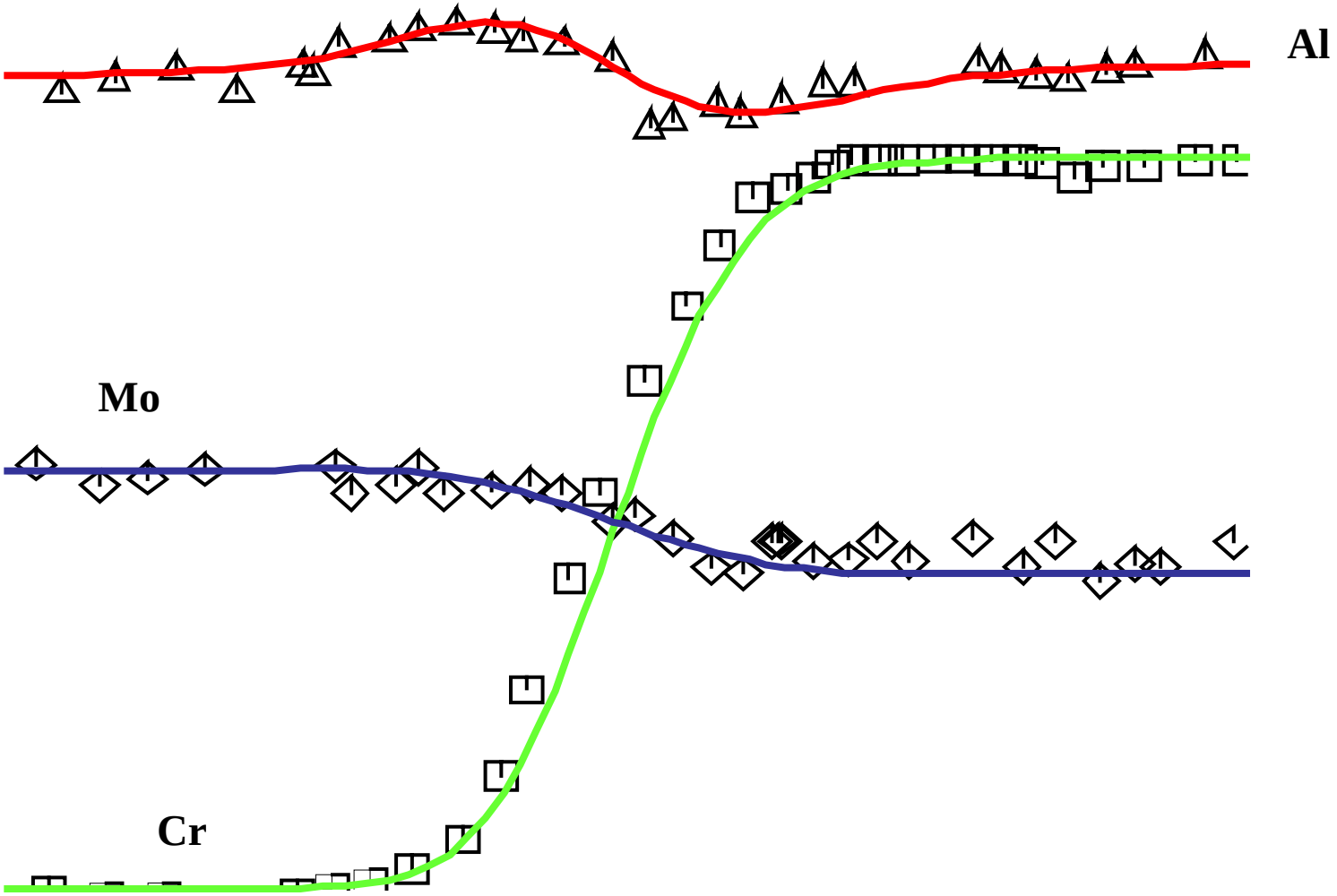
possible

- Determination of phase fractions
- Prediction of onset of precipitate formation
- Determination of temperatures for phase transitions
- Estimation of solidification behaviour
- Determination of thermodynamic data

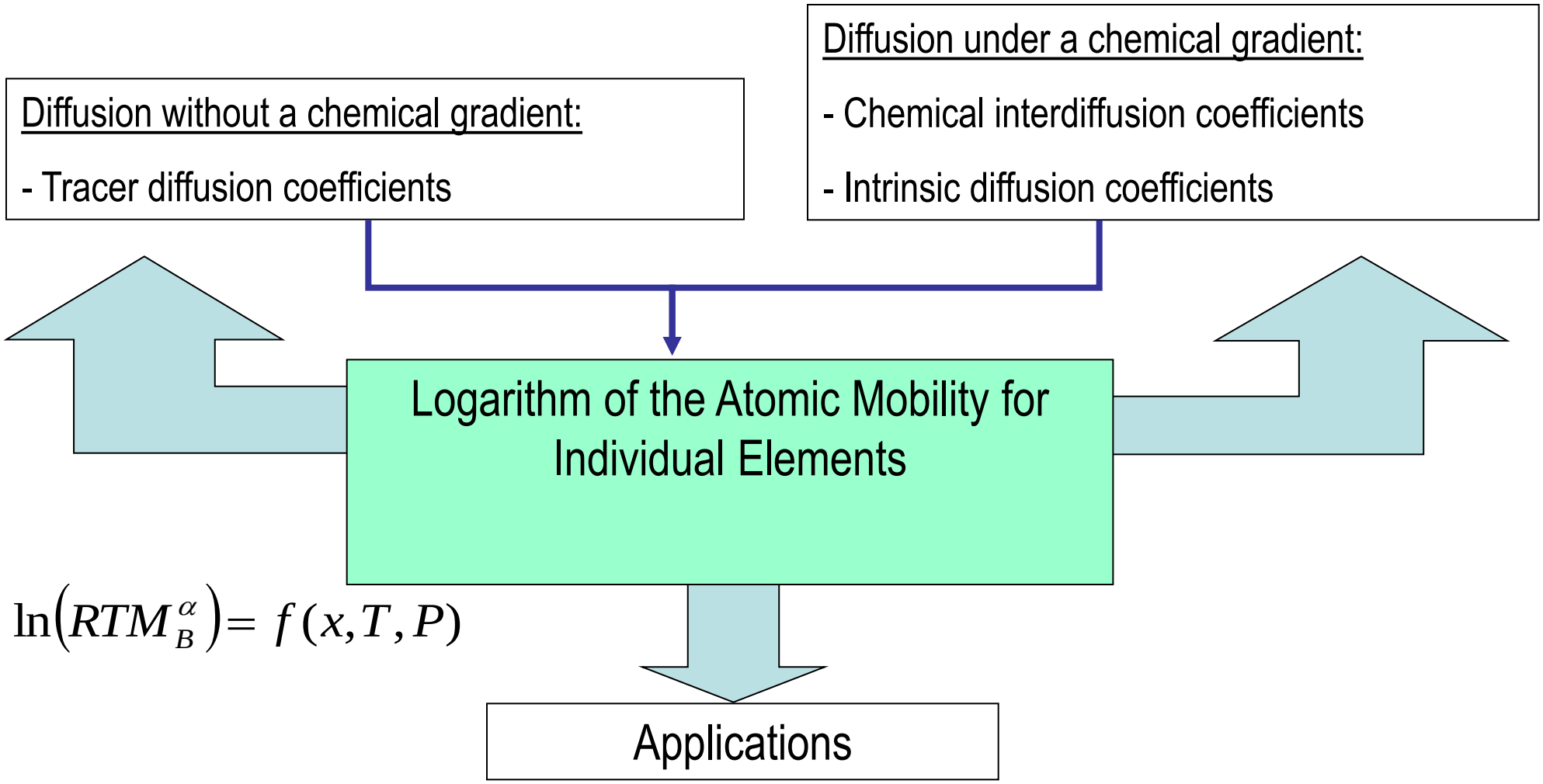
Not available

- Information on kinetics
- Information on microstructure
- Information about materials properties

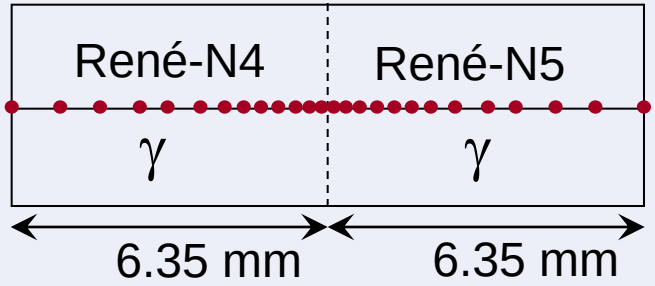
DICTRA: Diffusion Controlled TRAnsformations



Databases for diffusion coefficients/mobilities



Interdiffusion in complex alloy systems



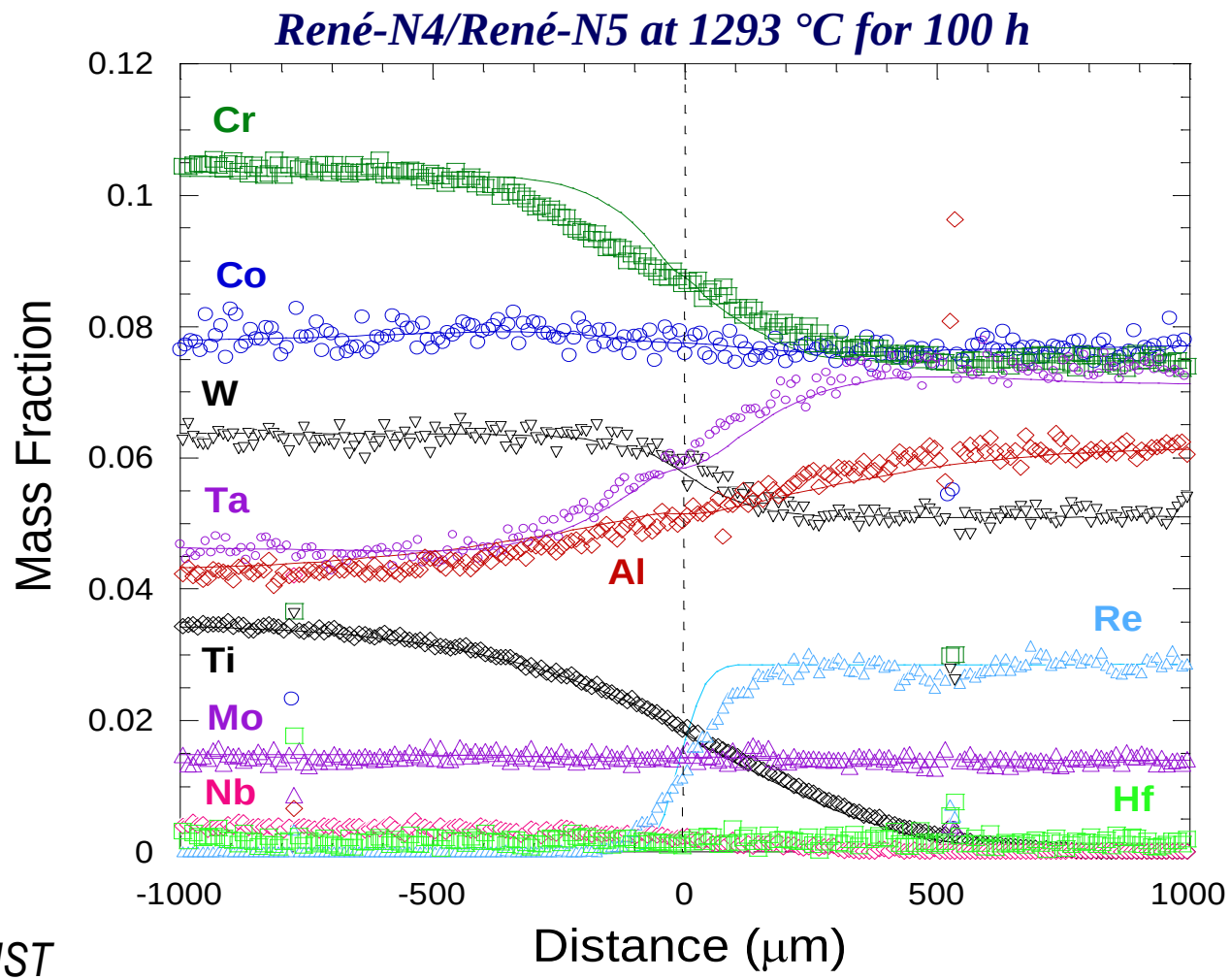
Double geometric grid: 200 points

Databases used

Thermodynamics: ThermoTech

Kinetics: NIST Ni-mob

D is a 10×10 matrix where all coefficients depend on concentration



From: C. E. Campbell, Metallurgy Division, NIST

Experimental work performed by T. Hansen, P. Merewether, B. Mueller, Howmet Corporation, Whitehall, MI.

Intermediate summary 2

possible

- Determination of phase fractions
- Prediction of onset of precipitate formation
- Determination of temperatures for phase transitions
- Estimation of solidification behaviour
- Determination of thermodynamic data
- Information on kinetics (diffusion)

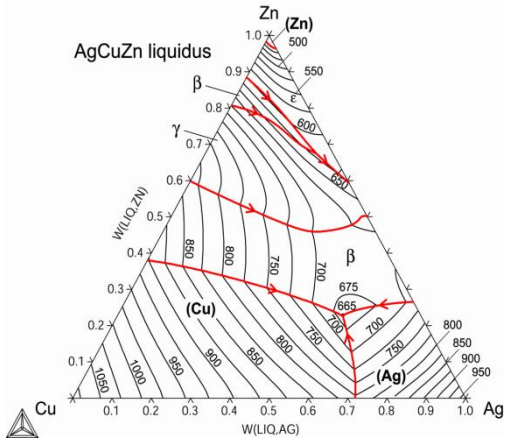
still not available

- Information on microstructure
- Information about materials properties

Mechanisms of microstructure evolution

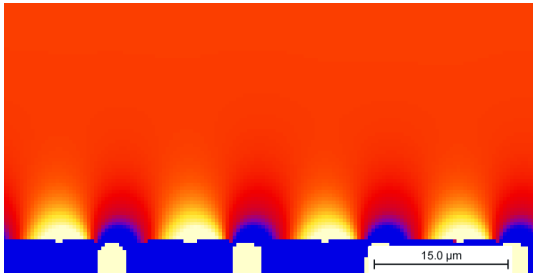
microstructure formation

thermodynamics (energy scale)



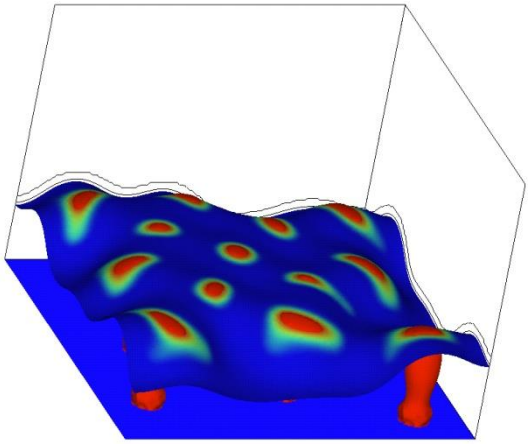
+

transport / diffusion (time scale)



+

interfaces (length scale)



TQ interface from TCS

diffusion solver

phase field method

micress®

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www.micress.de

access

Theories of phase transitions/ Phase-field models

van der Waals (1893)

Korteweg (190

Landa

Cahn

Halper **'7)**

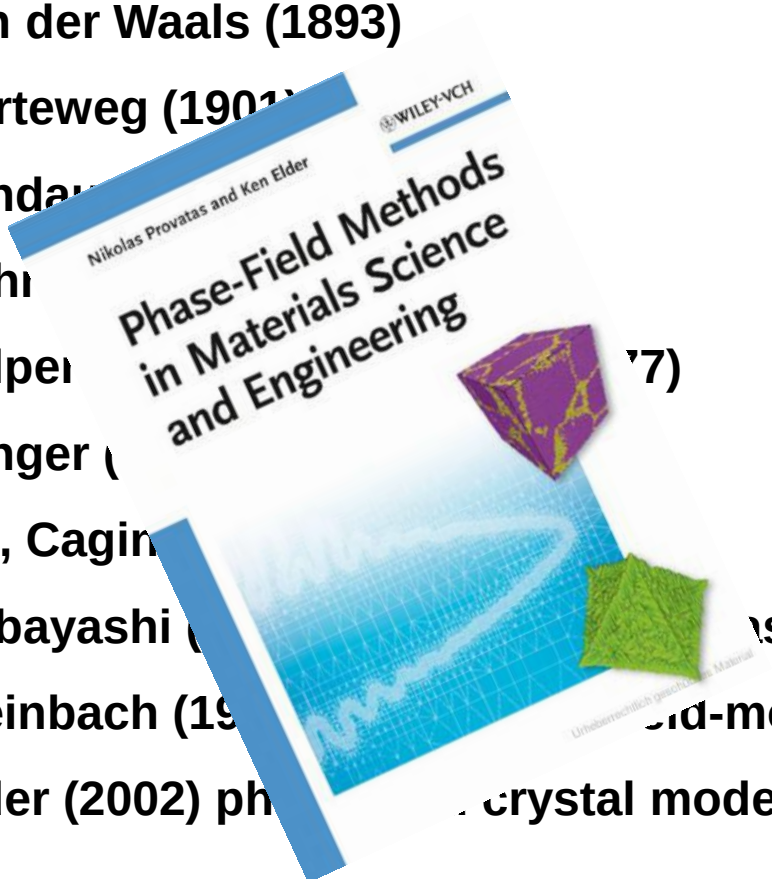
Langer (

Fix, Cagin

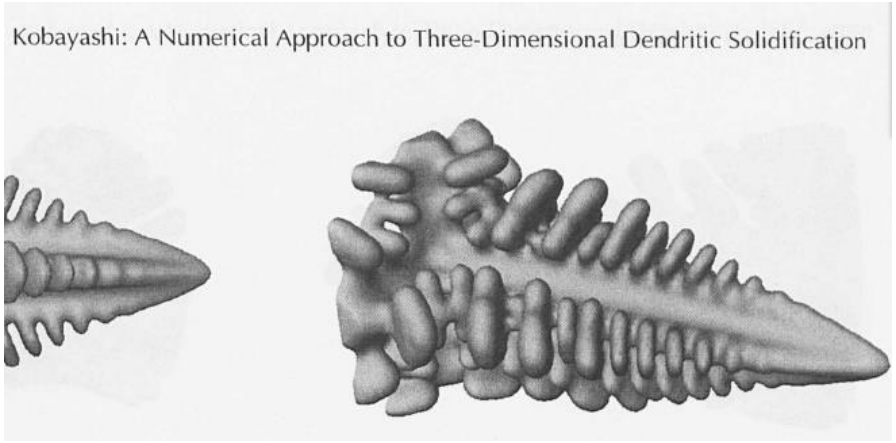
Kobayashi (**se field**

Steinbach (19 **d-model**

Elder (2002) ph **crystal models**



2010



PHYSICA D

Physica D 94 (1996) 135–147

A phase field concept for multiphase systems

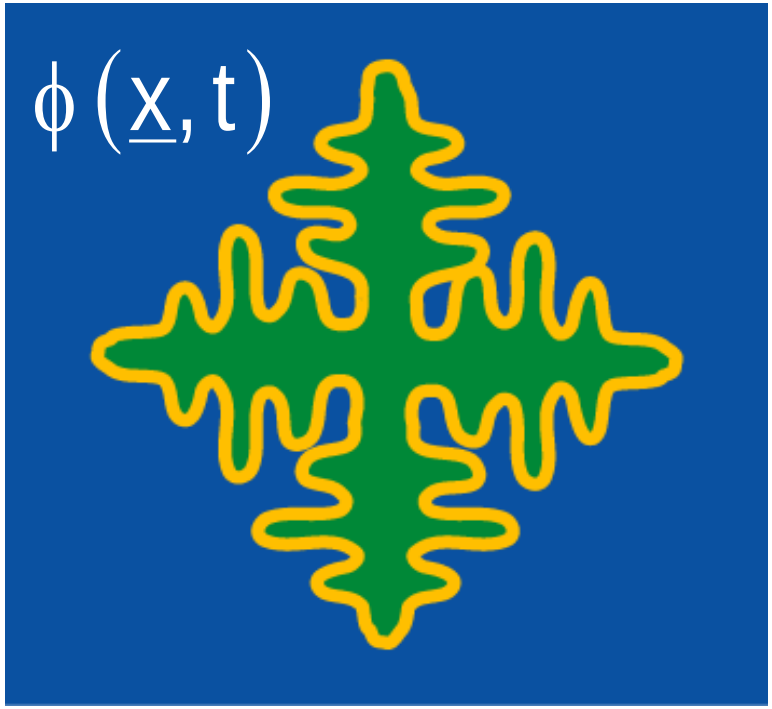
I. Steinbach [a,*], F. Pezzolla [a], B. Nestler [a], M. Seeßelberg [a], R. Prieler [a], G.J. Schmitz [a], J.L.L. Rezende [b]

[a] *ACCESS e.V., Intzestraße 5, D-52072 Aachen, Germany*
[b] *Foundry Institute RWTH Aachen, D-52056 Aachen, Germany*

Received 20 November 1995; accepted 30 November 1995
Communicated by H. Müller-Krumbhaar

Physica D 94 (1996)135

The phase-field model



Interpretation:

$\Phi(\underline{x}, t)$ corresponds to the fraction of a specific phase present at spot $\underline{x}$ and at time t

- $\Phi(\underline{x}, t) = ???$

Example solidifcation:

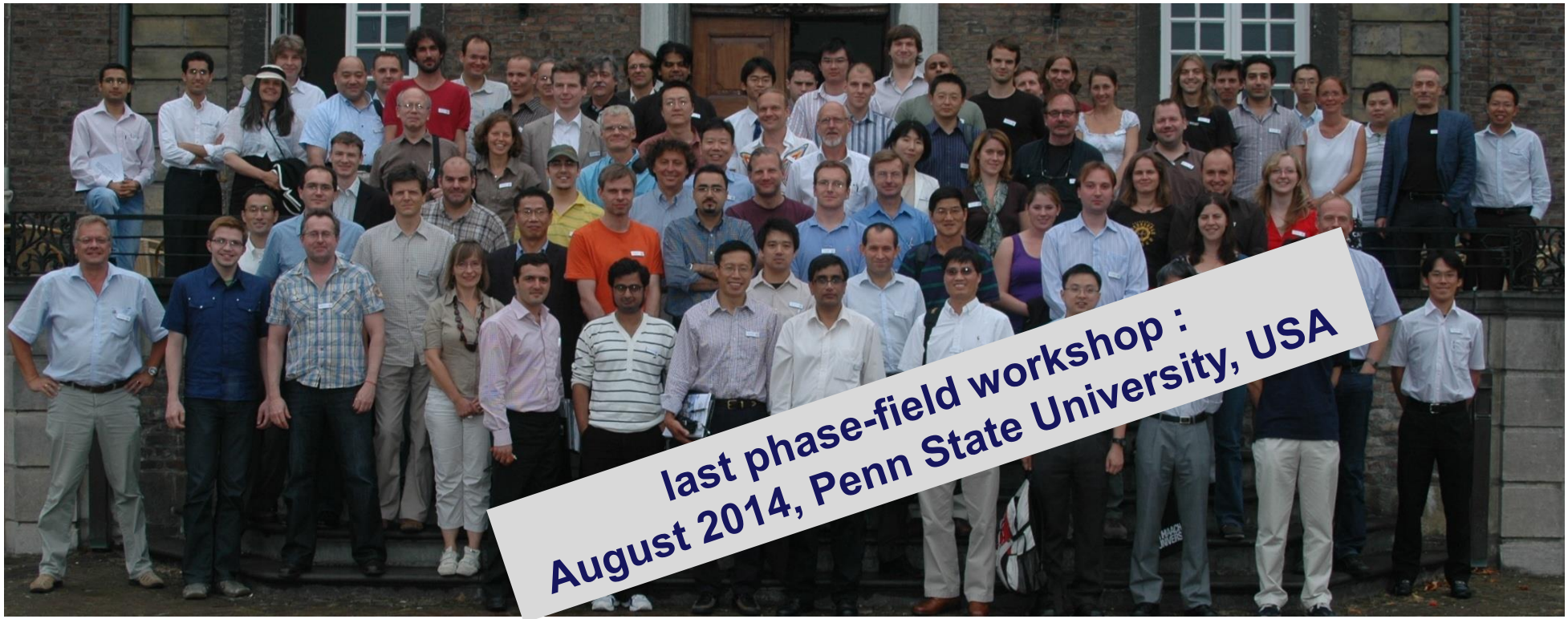
Φ corresponds to fraction „solid“:

: $\Phi(\underline{x}, t)$ equals 1 : 100 % solid 0 % liquid

: $\Phi(\underline{x}, t)$ equals 0 : 0 % solid 100 % liquid

: $\Phi(\underline{x}, t)$ between 0 and 1 : diffuse boundary

The phase-field equation(s) .....an own area of research

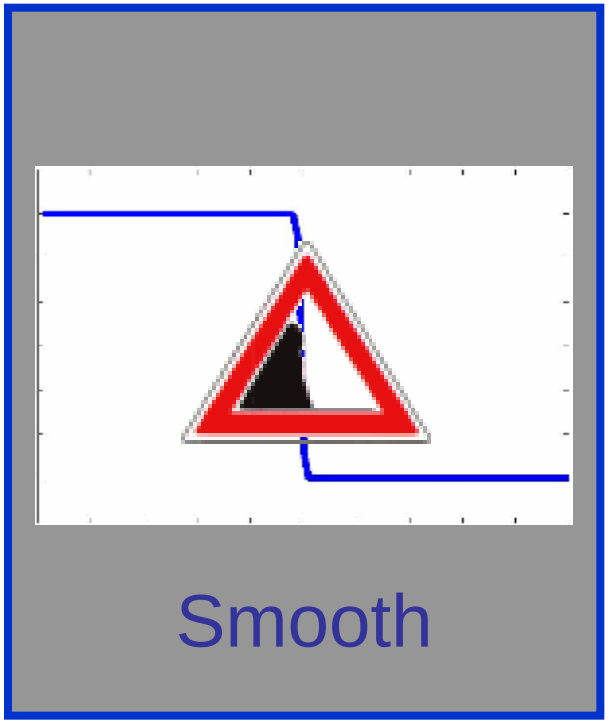


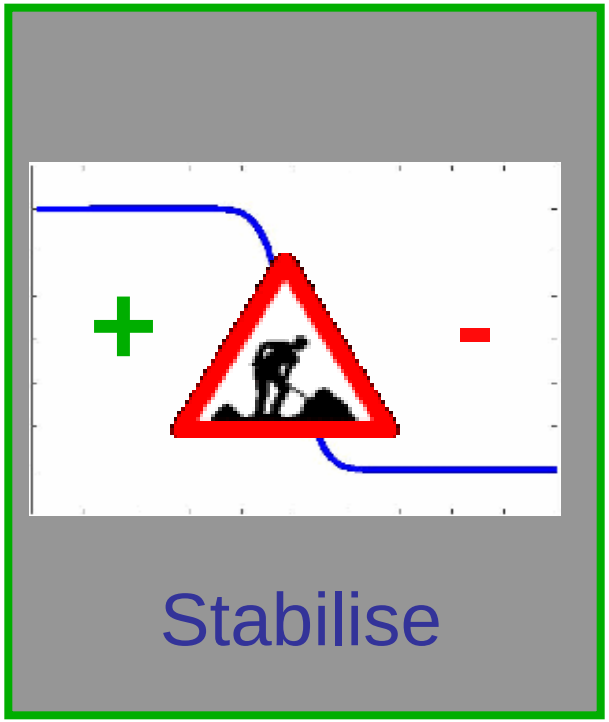
2nd International Symposium on
Phase-Field Modelling in Materials Science
Aachen, Germany, 2009

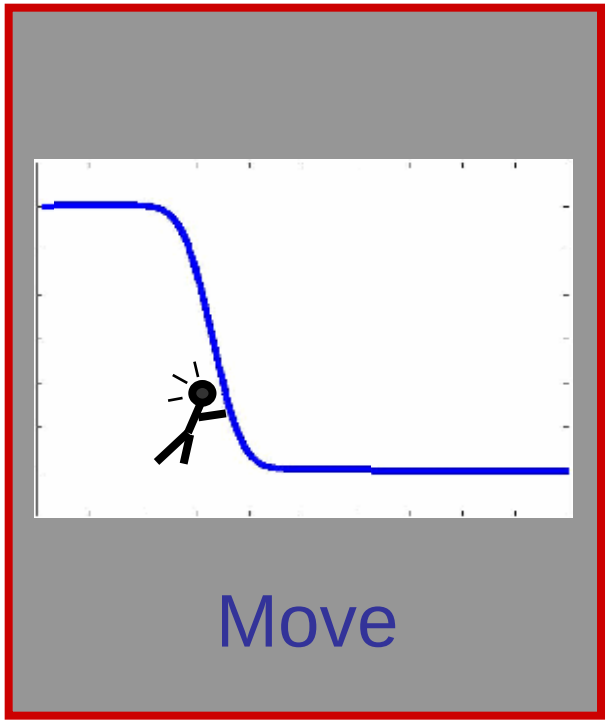
The phase-field equation

a very simple analysis (graphics: courtesy Nils Warnken, University of Birmingham)

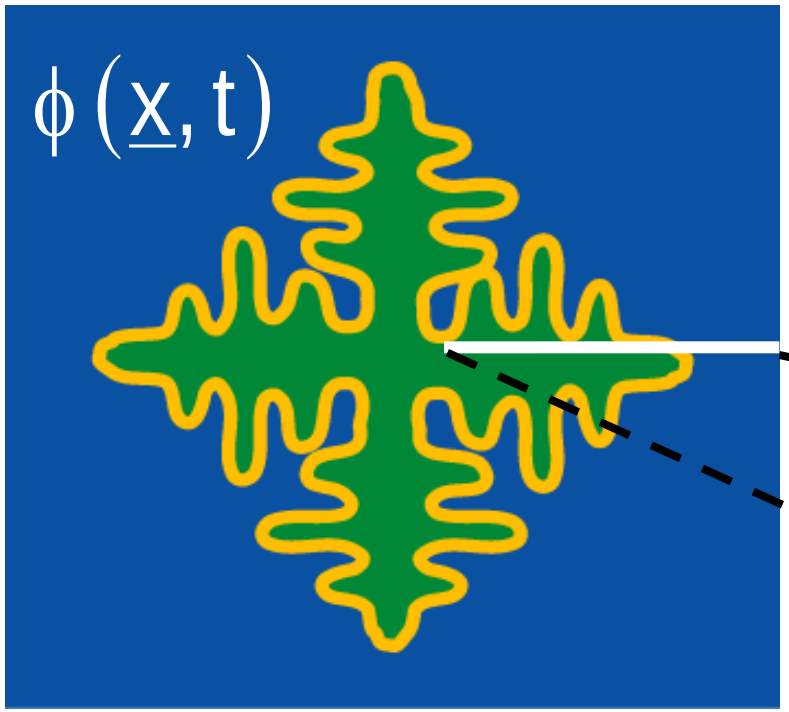
$$\dot{\phi}_s(\vec{x},t) = \mu\left[\sigma\left(\nabla^2\phi_s - \frac{(1-\phi_s)(1-2\phi_s)\phi_s}{\delta^2}\right) + \frac{1}{\delta}\Delta G\,\phi_s(1-\phi_s)\right]$$



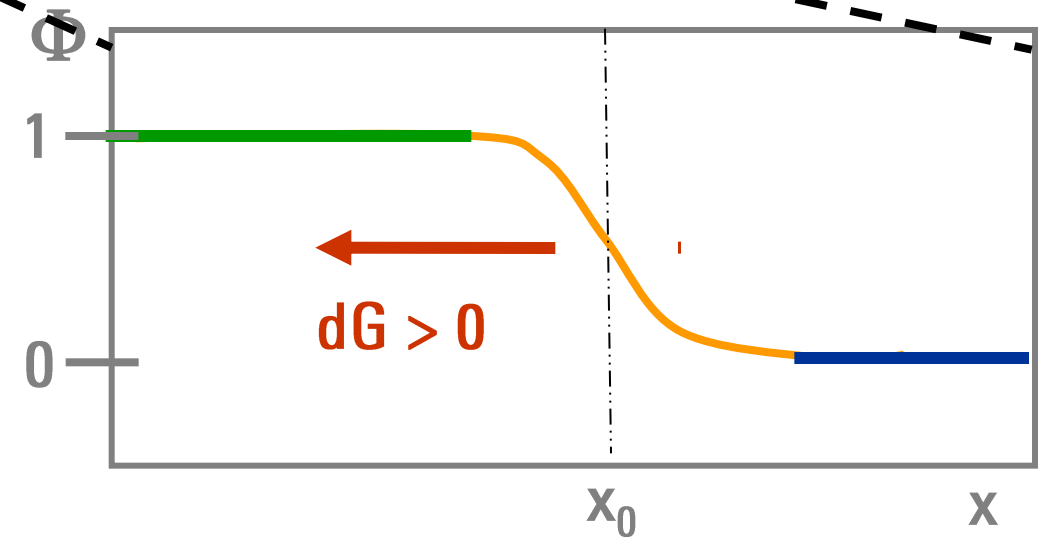




The Phase-Field Model



A PDE describes the evolution of the phase-field $\Phi(\underline{x}, t)$. The stationary solution describes the profile of the – diffuse- interface

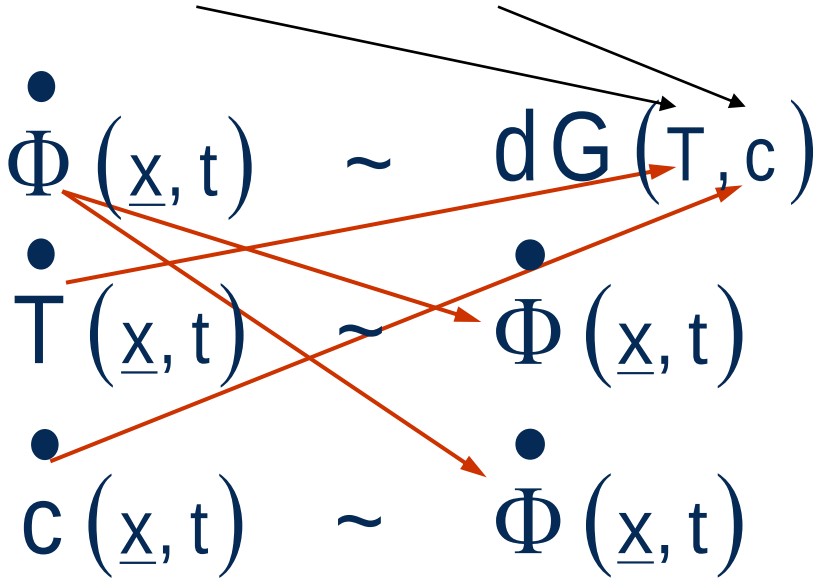


Depending on local coditions at the interface there is a driving force dG for

growth (dG <0)
or dissolution (dG >0)

The driving force

The driving force dG depends on local conditions of external fields (e.g. temperature, concentration, but also: elastic strains, electric or magnetic fields,…)



dG drives the evolution of the phase-field

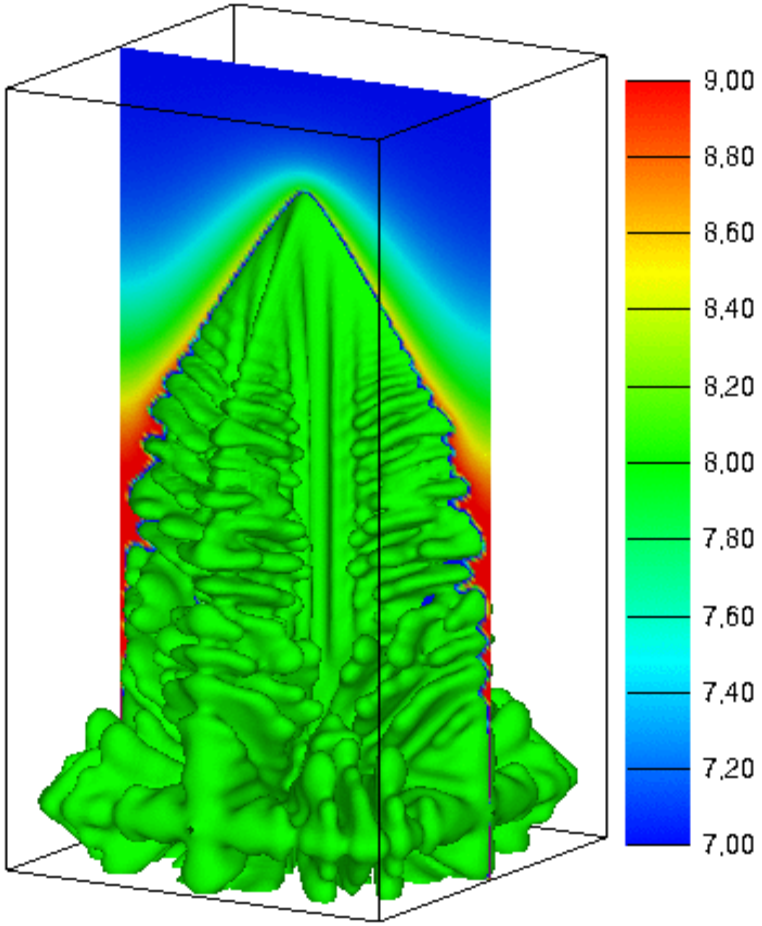
solidifying fractions release latent heat and thus influence the temperature field

..and – due to segregation– also the evolution of the solutal field

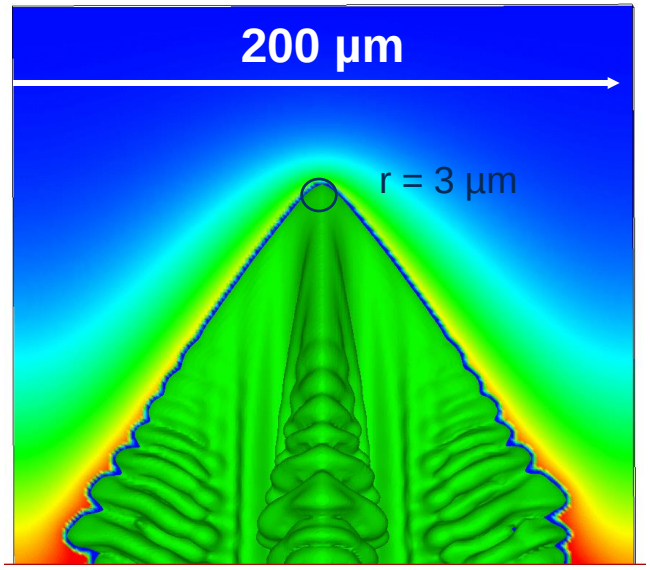
Coupling all these effects….

….leads to evolution of complex structures and patterns when numerically iterating such systems of coupled PDE's

solutal dendrite in Al-Si7 in 3 -dimensions



temperature gradient:∇ T = 20 K/mm
solidification velocity: v = 5 mm/s

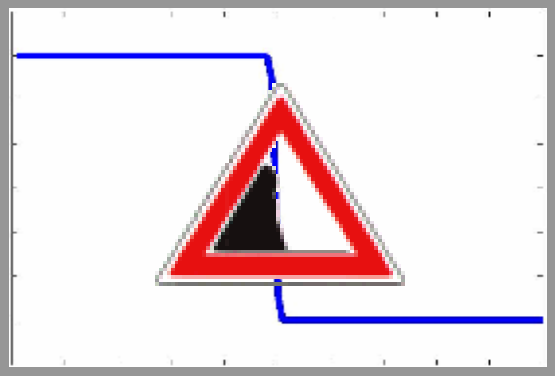


The phase-field equation

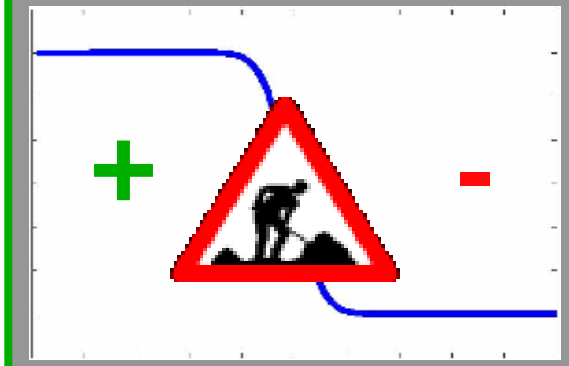
a very simple analysis (graphics: courtesy Nils Warnken, University of Birmingham)

$$[\mu = \mu_0(1-\cos(4\theta))] \quad [\sigma = \sigma_0(1-\cos(4\theta))]$$

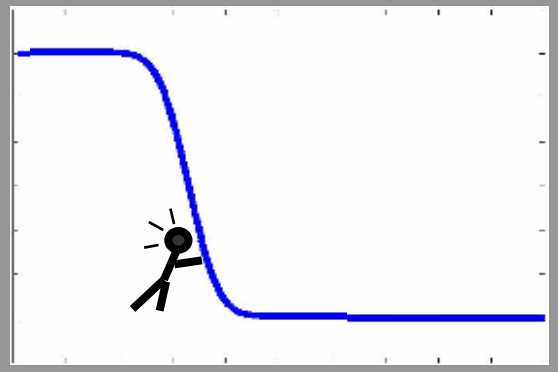
$$\dot{\phi}_s(\vec{x},t) = \mu\left[\sigma\left(\nabla^2\phi_s - \frac{(1-\phi_s)(1-2\phi_s)\phi_s}{\delta^2}\right) + \frac{1}{\delta}\Delta G\,\phi_s(1-\phi_s)\right]$$



Smooth



Stabilise



Move

Multiphase-Field Model for technical alloy systems

Technical alloys comprise:

- numerous grains
- numerous phases
- numerous elements

Their numerical description requires at least :

- multiple phase-fields
- description of diffusion in multicomponent systems
- thermodynamic databases

ELSEVIER

Physica D 94 (1996) 135–147

PHYSICA D

A phase field concept for multiphase systems

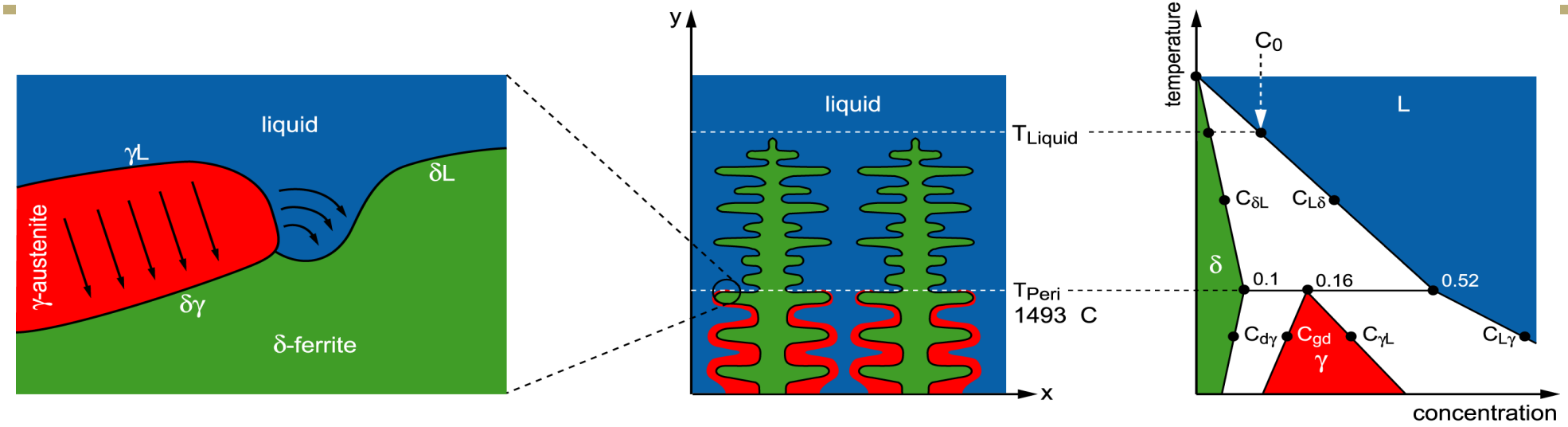
I. Steinbach [a,*], F. Pezzolla [a], B. Nestler [a], M. Seeßelberg [a], R. Prieler [a], G.J. Schmitz [a], J.L.L. Rezende [b]

[a] *ACCESS e.V., Intzestraße 5, D-52072 Aachen, Germany*
[b] *Foundry Institute RWTH Aachen, D-52056 Aachen, Germany*

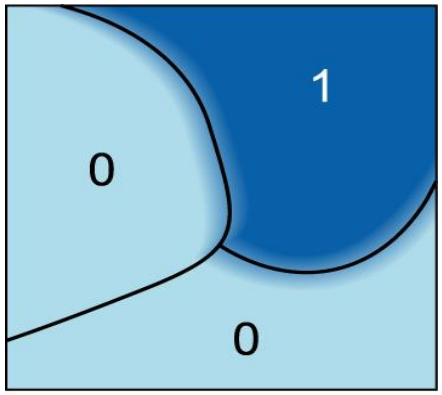
Received 20 November 1995; accepted 30 November 1995
Communicated by H. Müller-Krumbhaar

cited > 300 times (status Feb 2014)

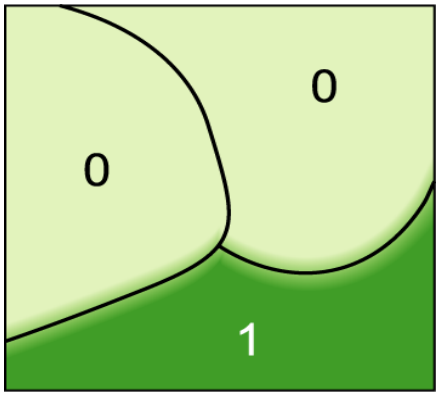
The Multiphase Field Method



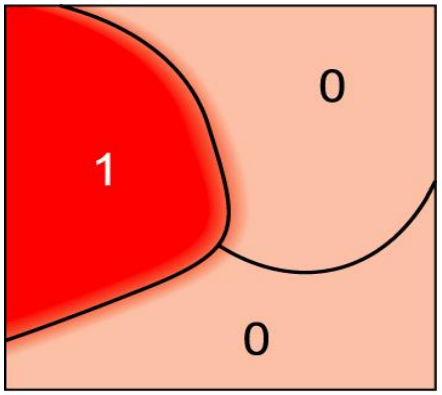
one phase field for each phase: $\phi_L + \phi_\delta + \phi_\gamma = 1$



ϕ_L



ϕ_δ



ϕ_γ

The Multi-Phase Field Approach

Basic ideas: *(see I.Steinbach et al. Physica D 94 (1996) 135)*

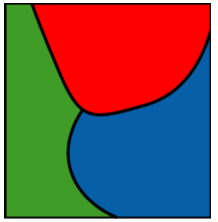
- definition of one phase field for each phase AND for each grain of a phase
- pairwise interaction for each pair of phases/grains like in standard phase-field
- possibility of implementation of specific phase/grain boundary properties

Further concepts:

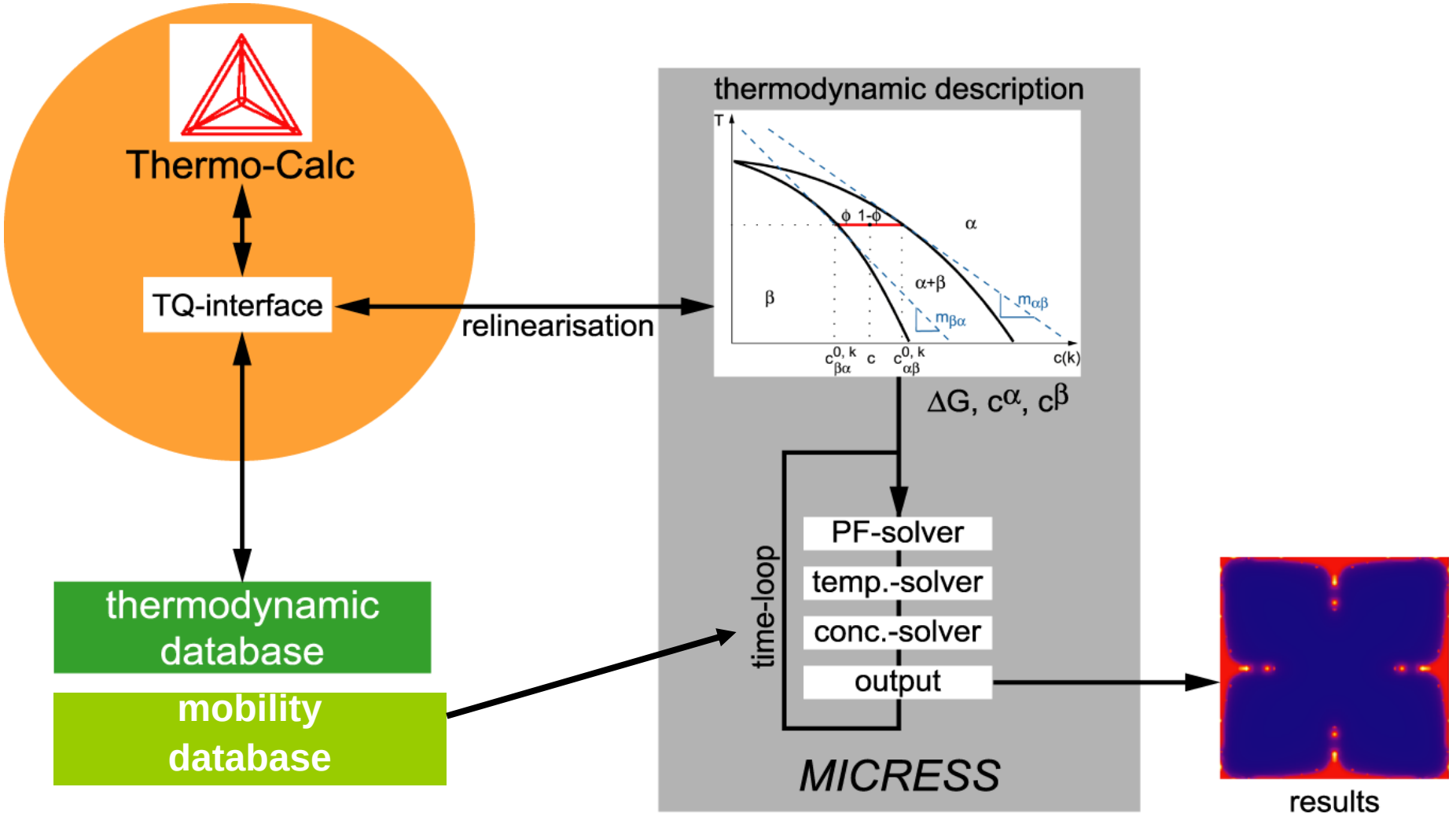
- coupling to thermodynamic databases
- coupling to mobility databases

Specific aspects:

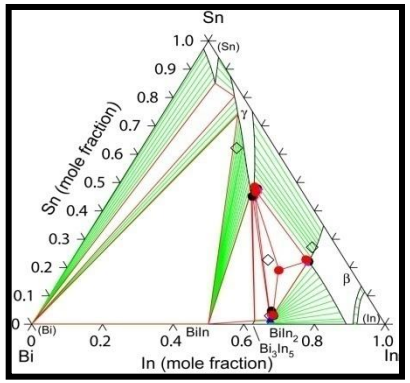
- 1D-simulation unable to reproduce multi-phase interactions
- physics of triple junctions



coupling to databases



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

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

temperature solver

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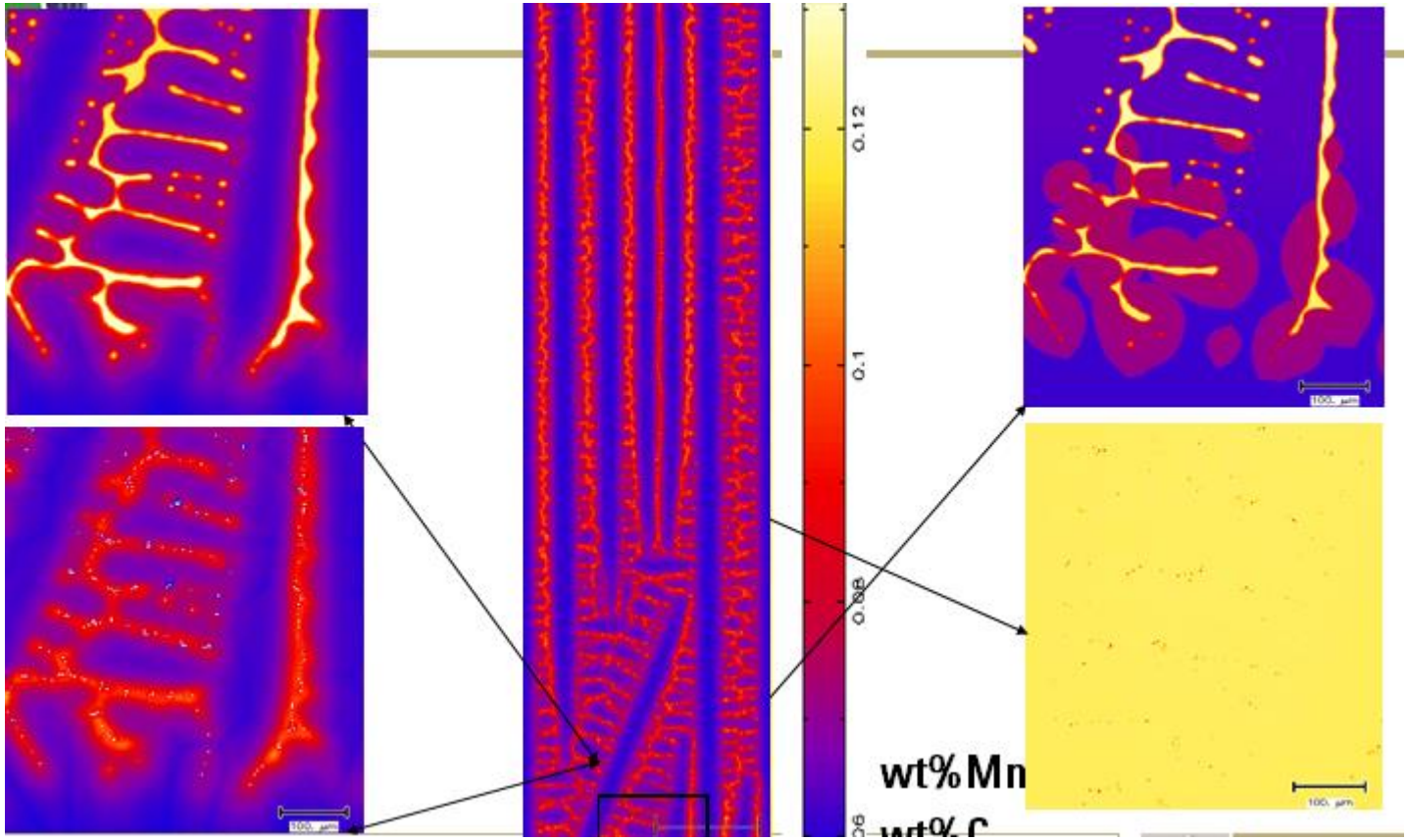
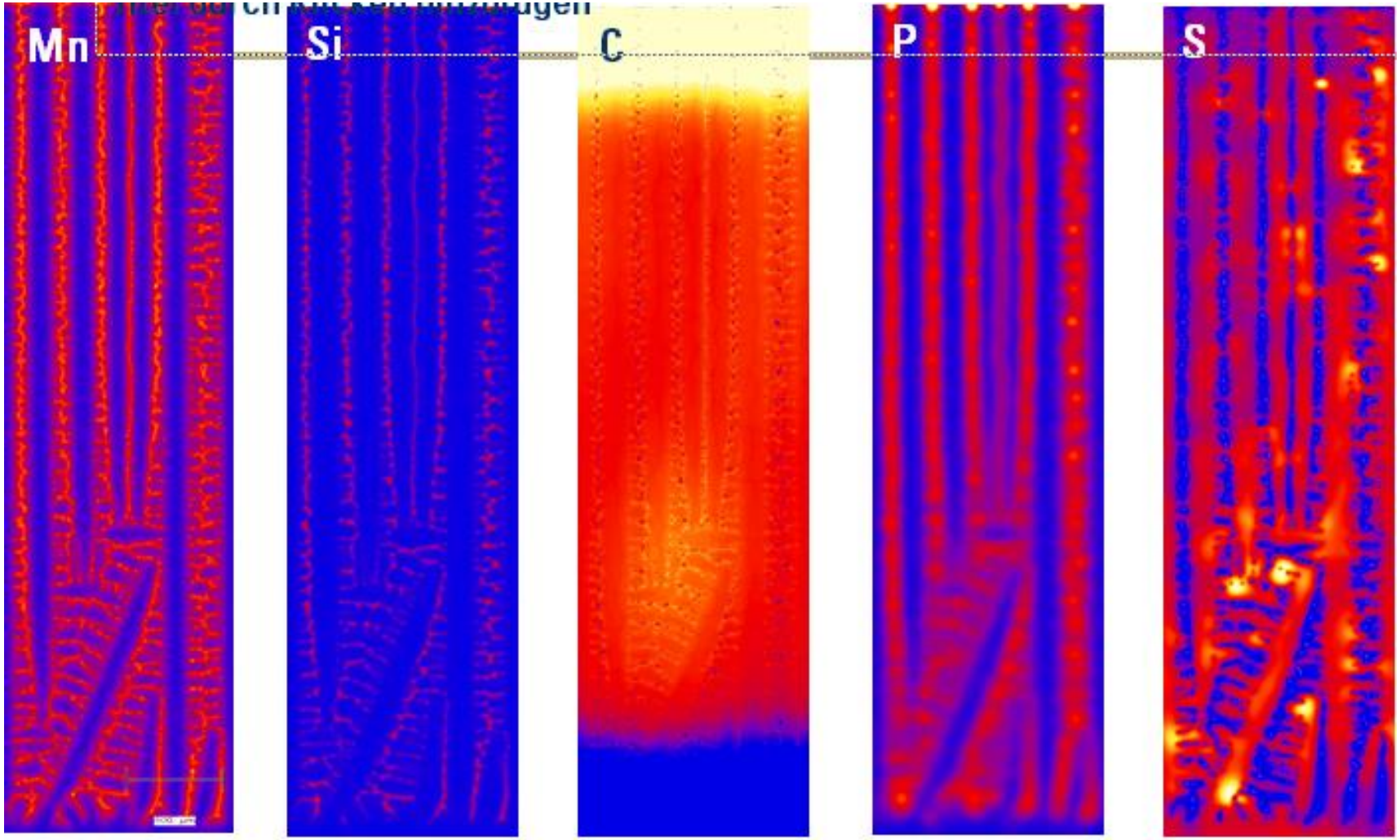
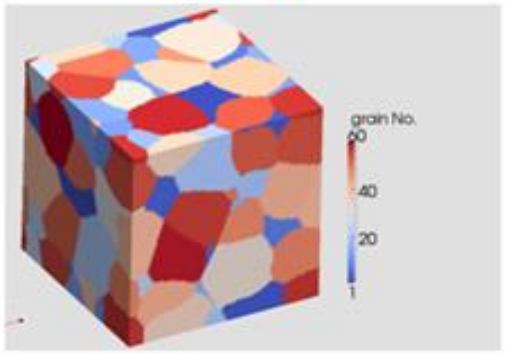
Directional Solidification



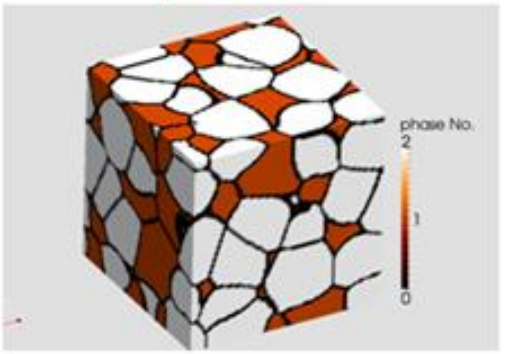

Mn
Si
C
P
S

Fe-C-Mn: stress and strain analysis during γ/α transformation

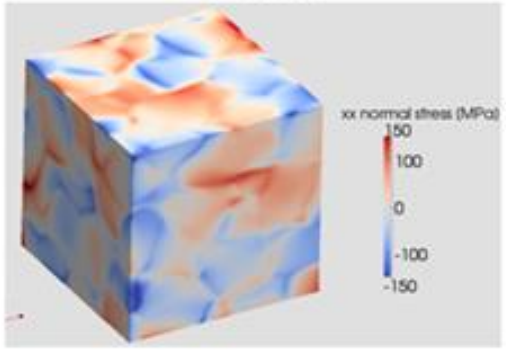
grain structure



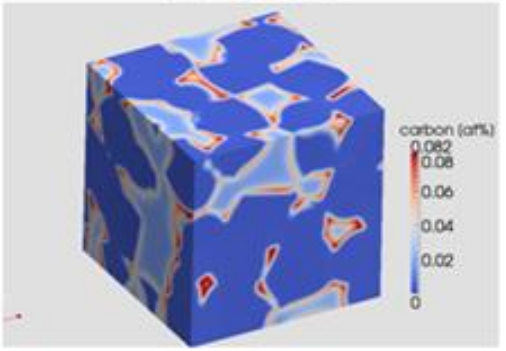
phase distribution



normal stress



carbon distribution



Intermediate summary 3

possible

- Determination of phase fractions
- Prediction of onset of precipitate formation
- Determination of temperatures for phase transitions
- Estimation of solidification behaviour
- Determination of thermodynamic data
- Information on kinetics
- Information on microstructure

still not available

- Information about materials properties
- Information about properties of component

Cluster of Excellence

Integrative Production Technologies for High Wage Countries

Virtual Process Chains for Processing of Materials

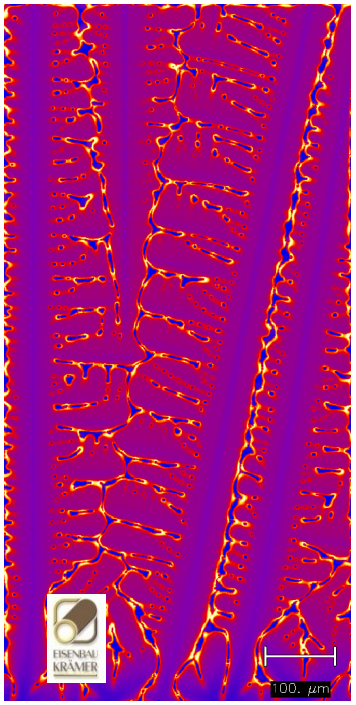
Speakers:

Dr.-Ing. Ulrich Prahl

Dr. rer.nat. Georg J. Schmitz

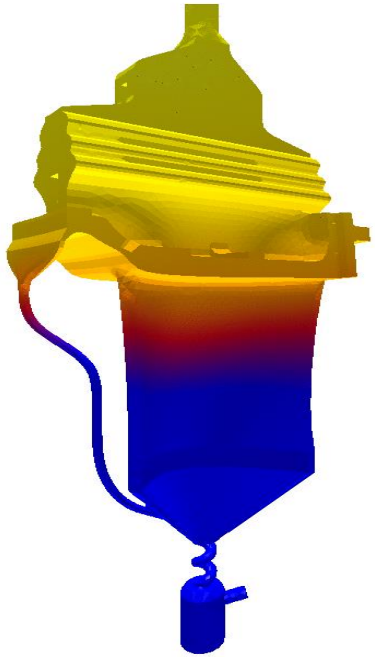
Virtual Process Chains for Processing of Materials

- casting - solidification - hot forming - cold forming - heat treatment - joining - coating -



Scopes

- integrative virtual description of processes and microstructure evolution along the production chain
- prediction of effective materials properties from calculated microstructures
- interfacing between microstructure simulations and macroscopic process simulations
- virtual documentation of the product history towards life cycle modelling
- verification for different test-cases of scientific and economic interest



Gießerei-Institut access IEHK ibf aachen ISF IOT ITA ILT Institut Lasertechnik Scientific Computing

staff involved (2013):

about 30 scientists (8 scientists full time equivalent)

AIXVIPMAP

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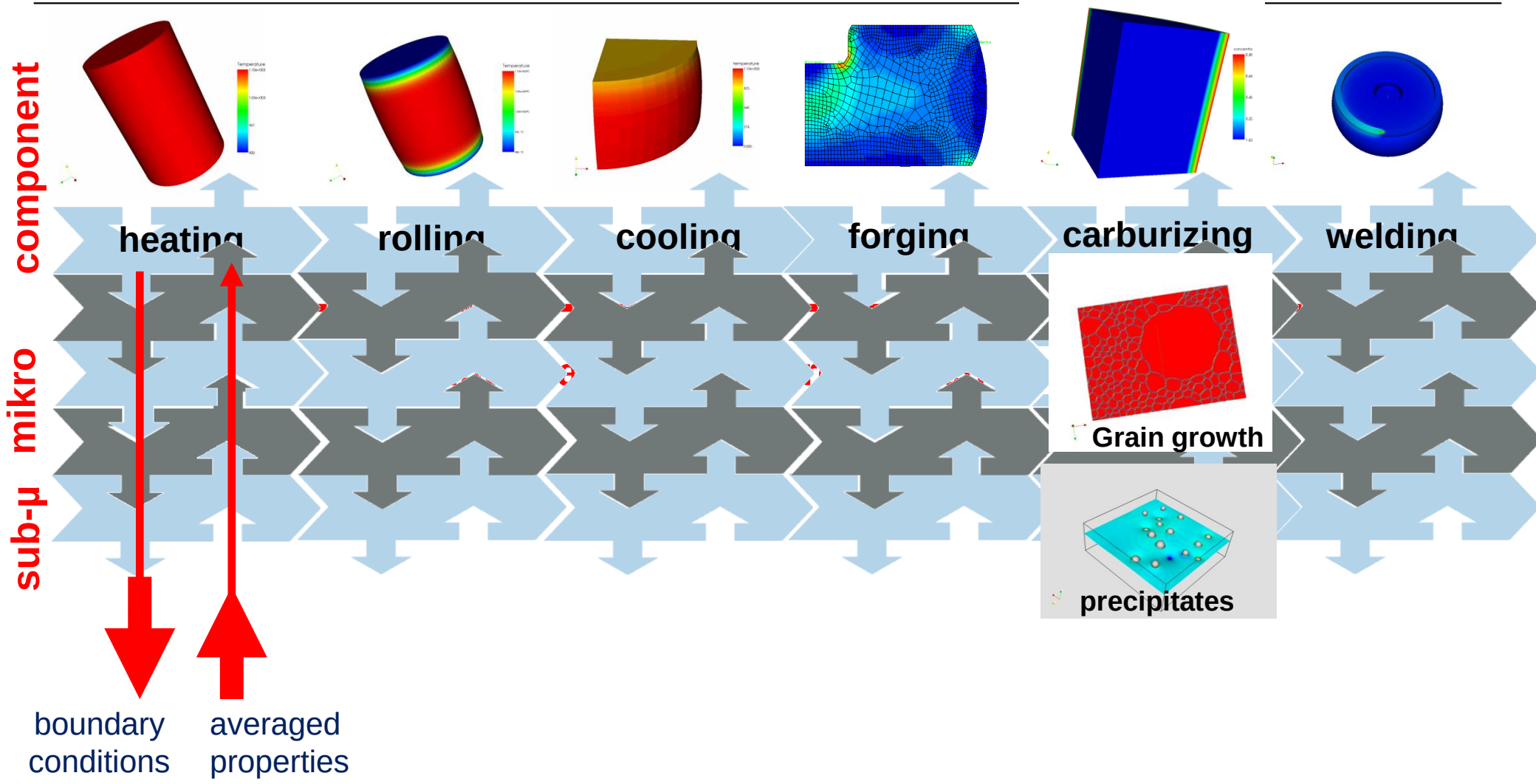
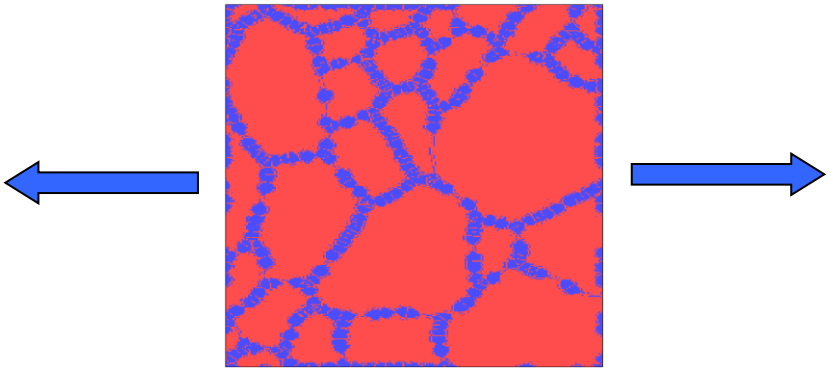
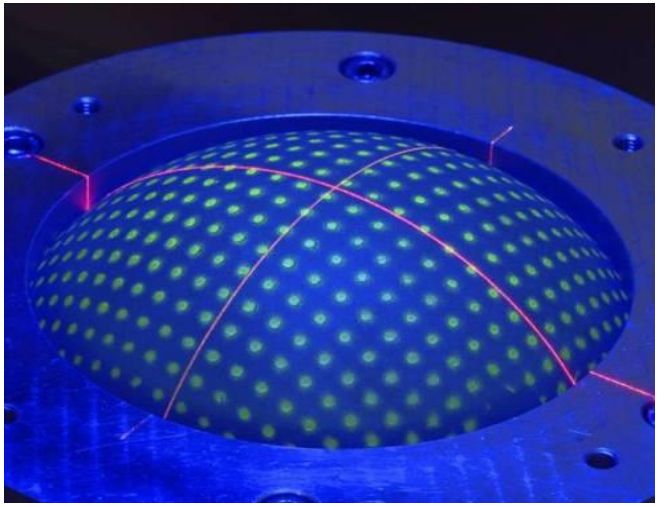
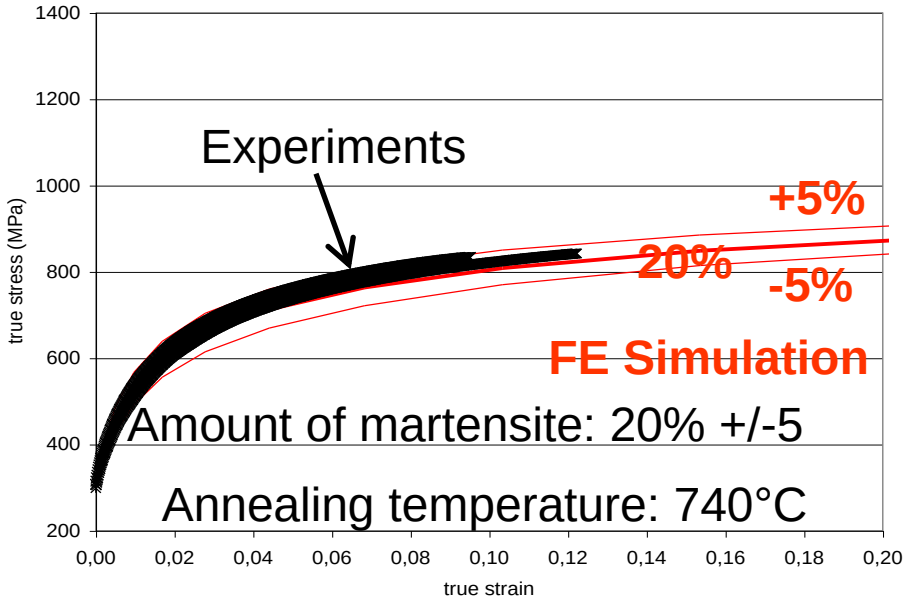
Example of a process chain



Numerical tensile tests







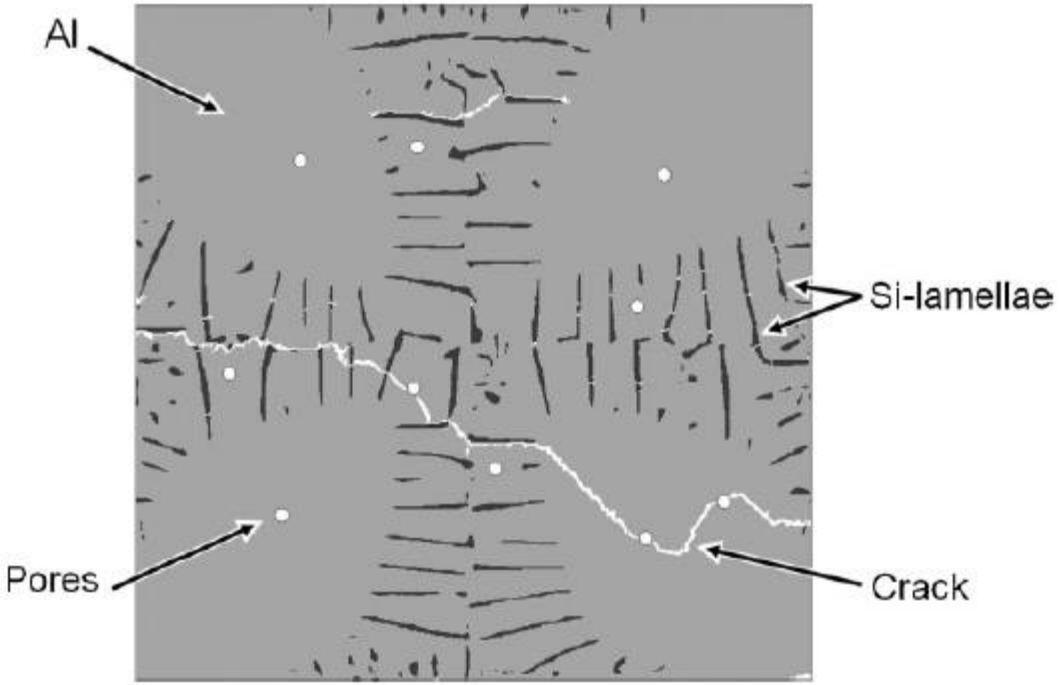
Numerical tensile tests of a simulated microstructure (DP600 steel) by means of RVE-FE and experimental bulge test show good agreement
PHD Thesis
C. Thomser IEHK RWTH Aachen (2009)

Crack propagation in virtual microstructure

DOI: 10.1002/adem.201100188

Effect of Microstructure and Hydrogen Pores on the Mechanical Behavior of an Al7%Si0.3%Mg Alloy Studied by a Combined Phase-Field and Micromechanical Approach**

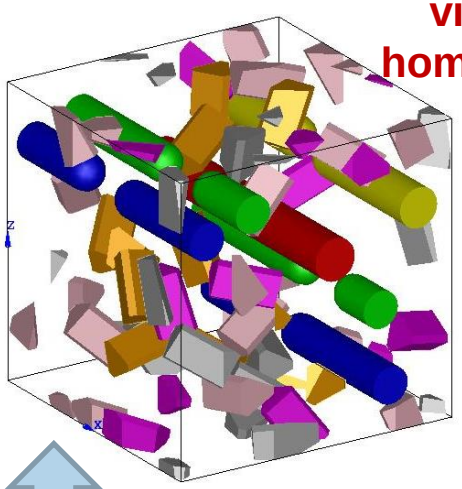
By *Galina Lasko,* Markus Apel, Antoine Carré, Ulrich Weber* and *Siegfried Schmauder*

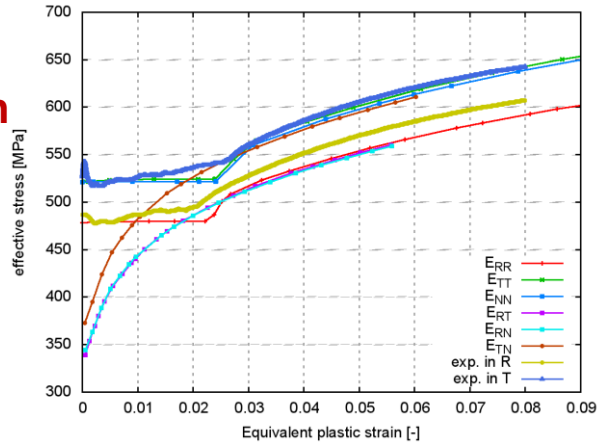


Effective properties

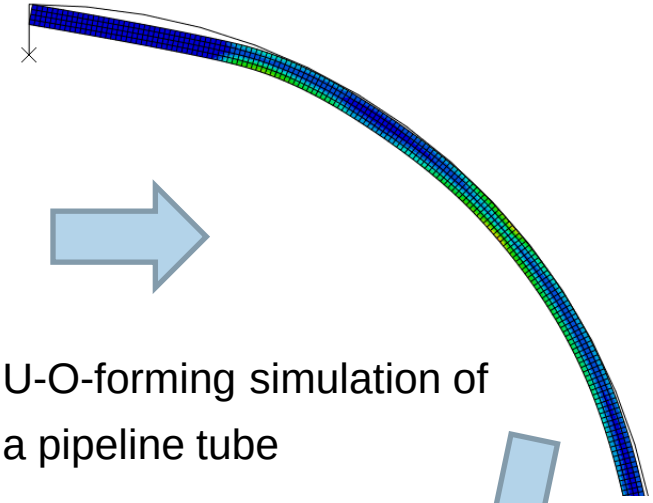
RVE: pearlite in ferrite matrix

virtual test/ homogenization

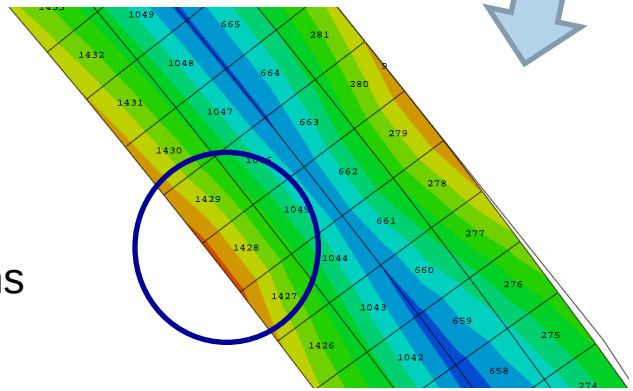




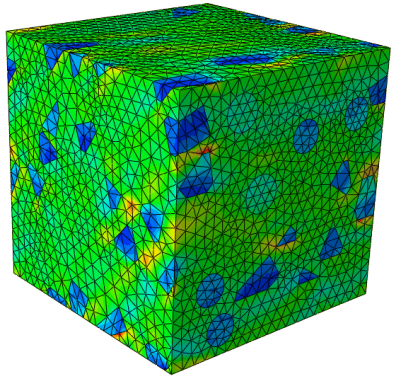
effective anisotropic flow curves



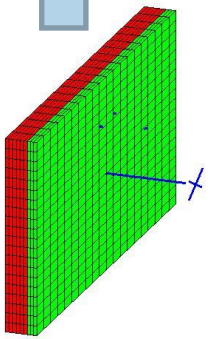
U-O-forming simulation of a pipeline tube



localization in critical regions:
applying local macrostrains on the RVE

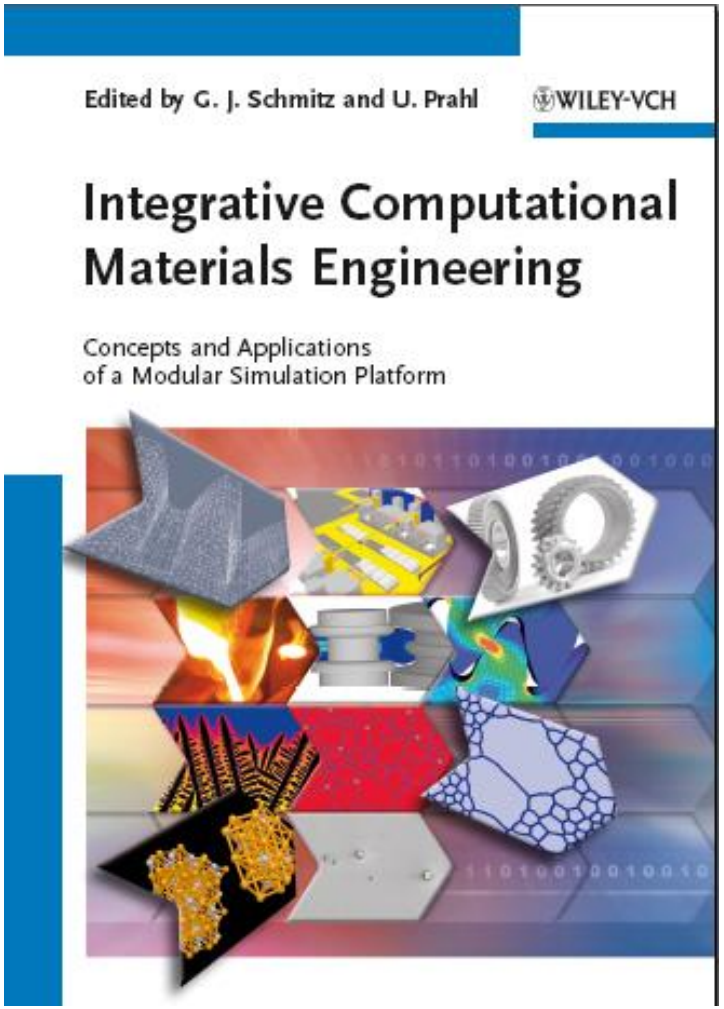


equivalent plastic microstrain



Ferrite-Cementite bilamella

…Integrated Computational Materials Engineering „ICME“….



appeared in April 2012

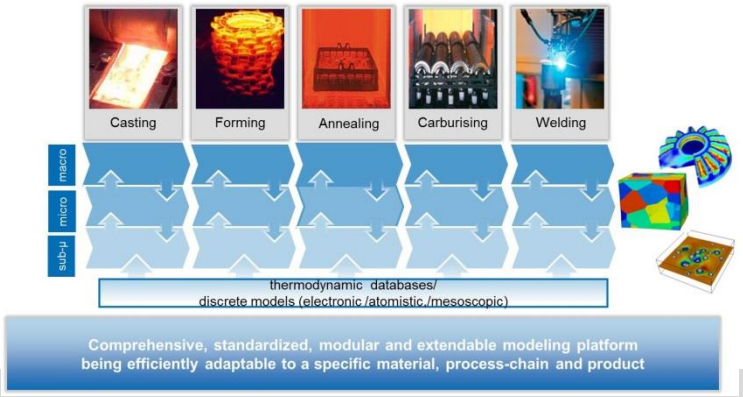
ISBN-10: 3-527-33081-X
ISBN: 978-3-527-33081-2

to appear in Chinese language edition in August 2016

The Integrated Computational Materials Engineering expert group - EU project ICMEg -

consortium: 11 partners, 6 countries

vision: plug&play in ICME



approach: global, open standards

How to do in practice? Read more:

ICMEg - the Integrated Computational Materials Engineering expert group - a new European coordination action

Integrating Materials and Manufacturing Innovation 2014, **3**:2 doi:10.1186/2193-9772-3-2

Georg J Schmitz (G.J.Schmitz@access.rwth-aachen.de)
Ulrich Prahl (Ulrich.Prahl@iehk.rwth-aachen.de)

www.icmeg.eu
www.icmeg.info

Final summary

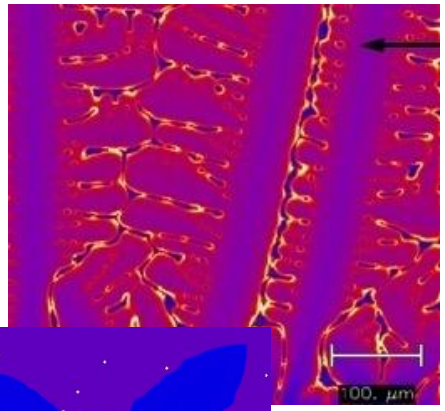
Possible/in reach

- Determination of phase fractions
- Prediction of onset of precipitate formation
- Determination of temperatures for phase transitions
- Estimation of solidification behaviour
- Determination of thermodynamic data
- Information on kinetics
- Information on microstructure
- Information about materials properties
- Information about properties of component
- Life cycle modelling

still not available

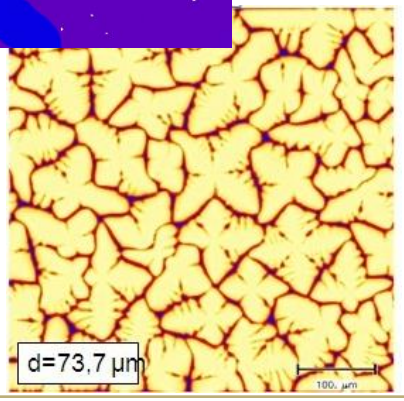
- Inverse modelling

MICRESS Simulations of technical alloy grades



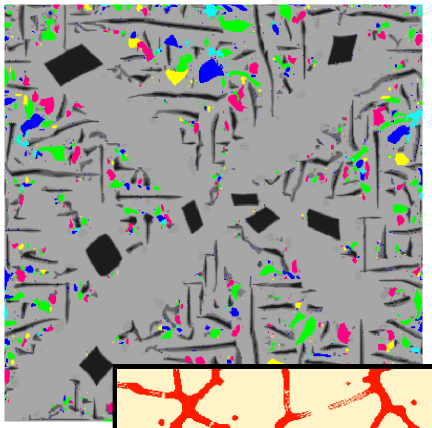
Steel
(e.g. stainless steel)

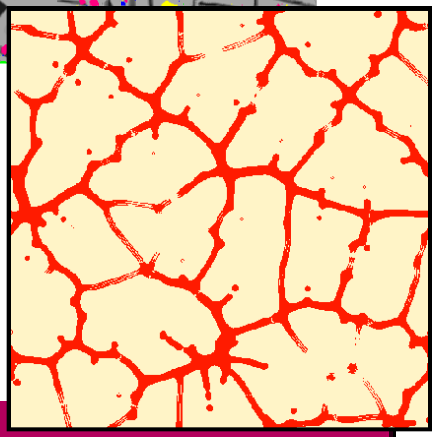
cast iron
(e.g. GJS)



Superalloys
(e.g. IN 718)

Al-alloys
(e.g. KS 1295)





Mg-alloys
(e.g. AZ 91)

Solders
(e.g. SAC)

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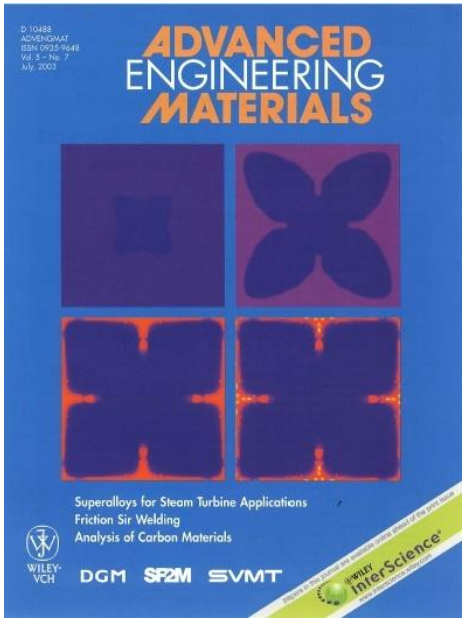
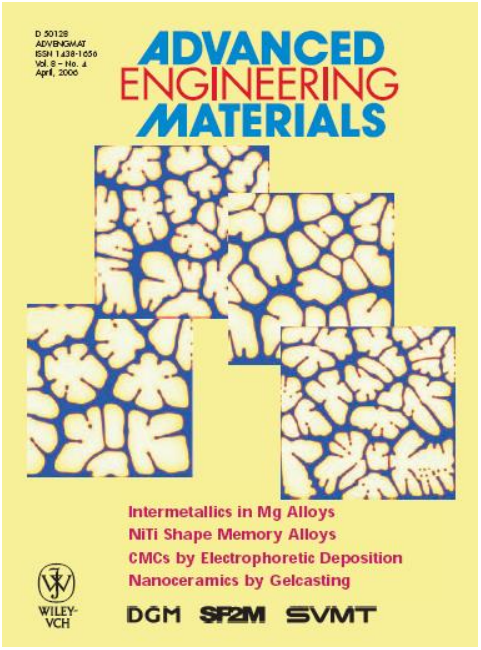
MICRESS in science…..



Adv.Eng.Materials 2003



Adv.Eng.Materials 2006

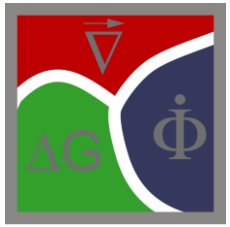
Adv.Eng.Materials 2009

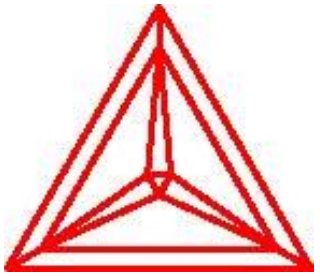
Int. J. Mater Res. 2010

Thanks!

Thank you very much for your attention!

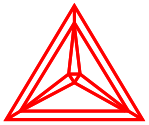
www.micress.de





Thermo-Calc Software

www.thermocalc.de
www.thermocalc.se



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