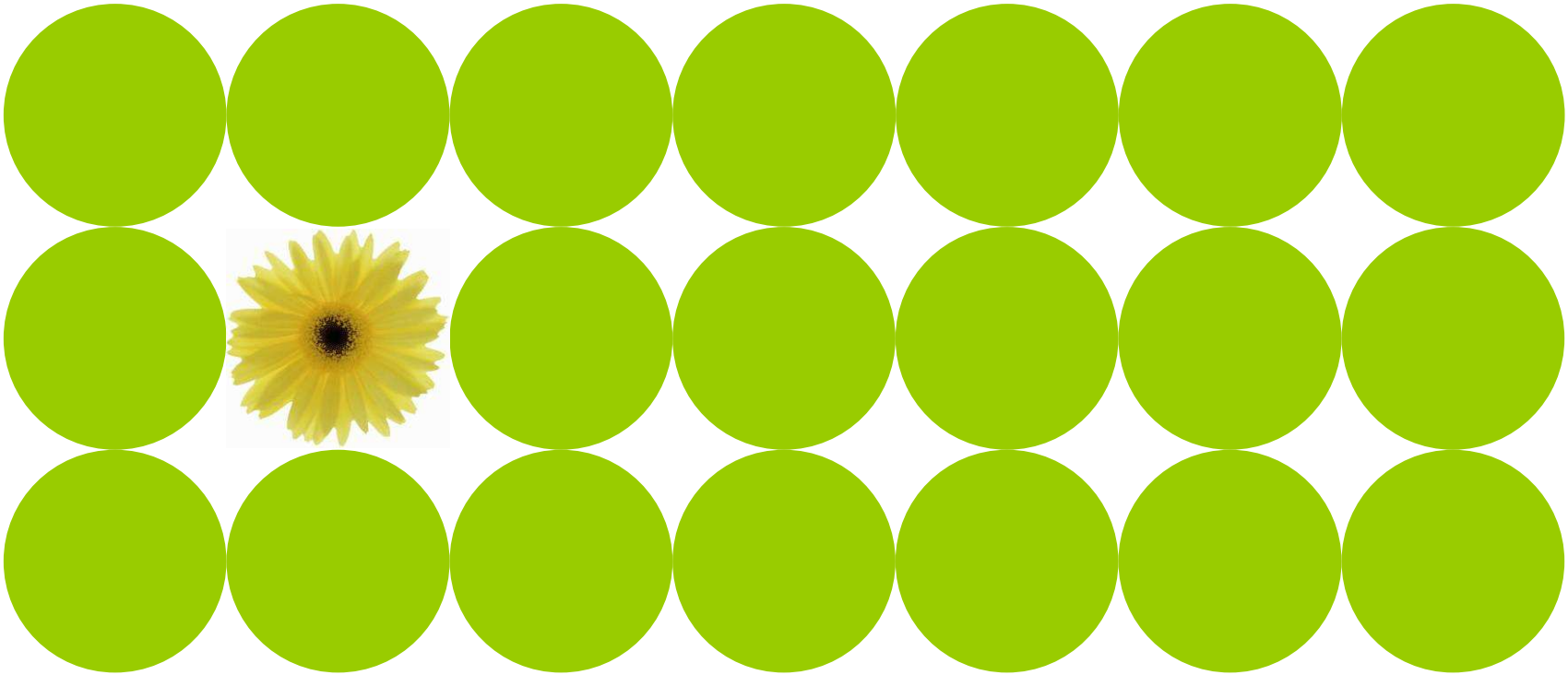
The Use of Computer Simulation of the Microstructure of Al-Alloys in Industrial Practice



Olaf Engler, Hydro RDB

GTT Workshop, Herzogenrath, 05.06.2008

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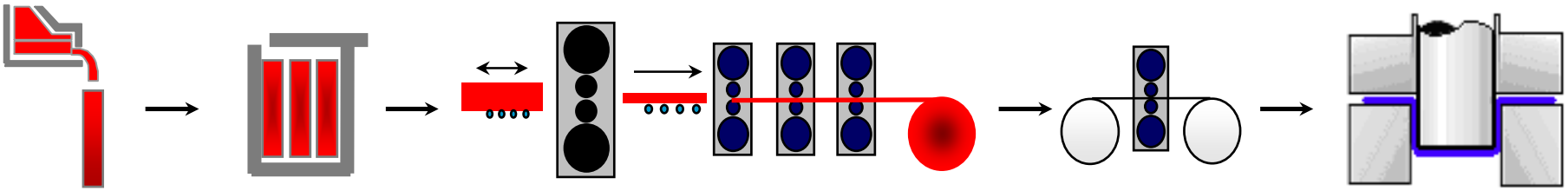
The Use of Computer Simulation of the Microstructure of Al-Alloys in Industrial Practice

Outline

- Introduction: through-process modelling
- Modelling Environment at RDB, incl. simulation of microchemistry
- Application example: thermostability in Al-foil



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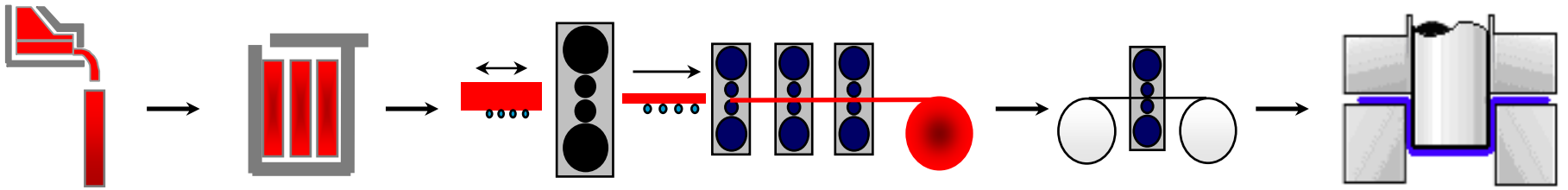
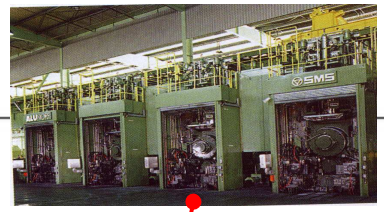
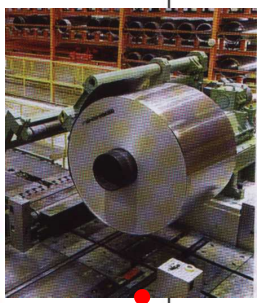


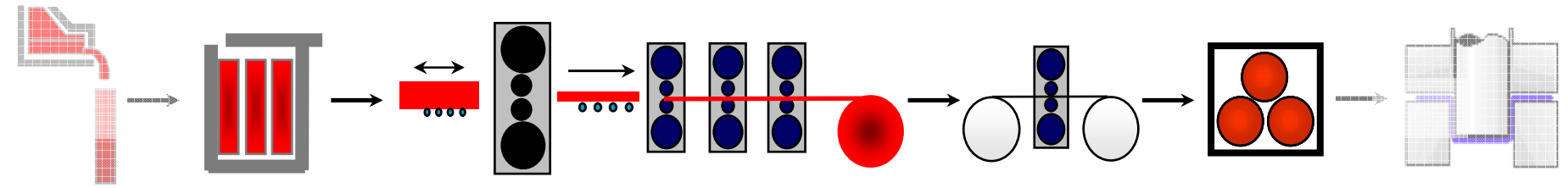




centre
surface
temperature in °C
500
450
400
350
300
Transport from Homogenising
Roughing mill (reversing)
Finishing mill (tandem)
Transport / Cropping
Coil
processing time

(3)

Through-Process Modelling



Main metallurgical reactions along the process chain

- **homogenisation:** diffusion, microchemistry (solutes, phases)
- **hot rolling:** work hardening, softening, texture, microchemistry
- **cold rolling:** work hardening, texture
- **back-annealing:** softening, texture

- microchemistry
- work hardening
- softening

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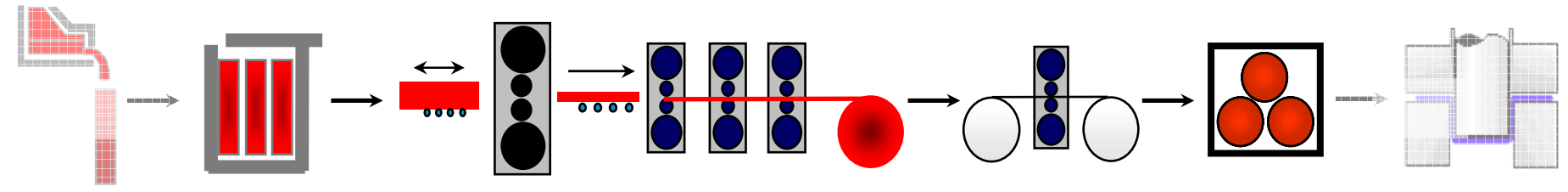
Through-Process Modelling



Modelling Environment at RDB

- microchemistry: FactSage (incl. Scheil), ClaNG
- work hardening: GIA, 3IVM
- softening: AlSoft

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BMBF Project ClaNG Plus

Duration:

- Start: 01.01.2007
- End: 31.12.2010

Partners

- Hydro Aluminium Deutschland GmbH, R&D Bonn – project management
- Institut für Metallkunde und Metallphysik, RWTH Aachen
- GTT-Technologies, Herzogenrath

Workpackages:

1) Model development ClaNG (IMM, Hydro)
2) Link of ClaNG model to modern multi component thermodynamic data bases (IMM, GTT, Hydro)
3) Link of ClaNG model to property models (IMM, Hydro)
4) Evaluation of applicability to solidification (IMM, Hydro)
5) Full scale trials and characterization (Hydro, IMM)

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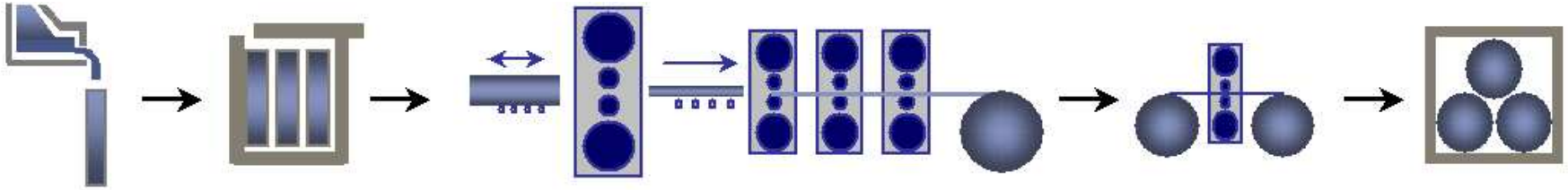
ClaNG Modell
"*Cla*ssical *N*ucleation and *G*rowth"



Process parameters
- time
- temperature
- dislocation density

Thermodynamic data
- alloy
- phase diagram
- diffusion coefficients
- interface energies

$$\Delta G(r_C) = \frac{4}{3} \cdot \pi \cdot r_C^2 \cdot \sigma$$

$$r_C = \frac{2 \cdot \sigma}{\Delta g_T}$$

$$\frac{dr}{dt} = \frac{c(t) - c^{\alpha}(r)}{c^{\beta} - c^{\alpha}(r)} \cdot 0.5 \cdot \frac{c(t) - c^{\alpha}(r)}{c^{\beta} - c(t)} \frac{D}{r}$$

$$N = N_0 \cdot Z \cdot \beta \cdot \exp\left(-\frac{\Delta G(r_C)}{k_B \cdot T}\right)$$

Micro-chemistry
- solute levels c_i
- particles $V_i(r)$
- type, size, volume

Input → ClaNG-Model → Output

ClaNG model overview

Goal: determine the precipitation kinetics

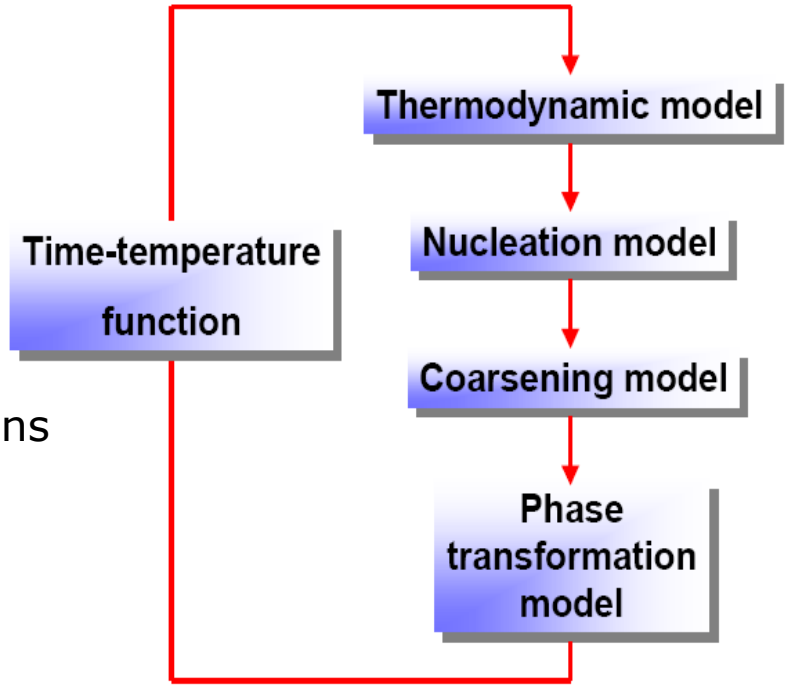
classical theories:

- Nucleation: *Becker and Döring*
- Growth: *Zener*
- Evolution of precipitate size distributions: continuity equation (*Kampmann and Wagner*)

Decision based on thermodynamic calculations using ChemApp (*GTT Technologies*)

- Data base: *Thermotech AlTT* (8 elements: Al-Cr-Cu-Fe-Mg-Mn-Si-Ti)

developed by L. Löchte (RDB), G. Gottstein (IMM) and M. Schneider (Diss. IMM, 2006), advanced by E. Jannot (Diss. IMM, 2008)



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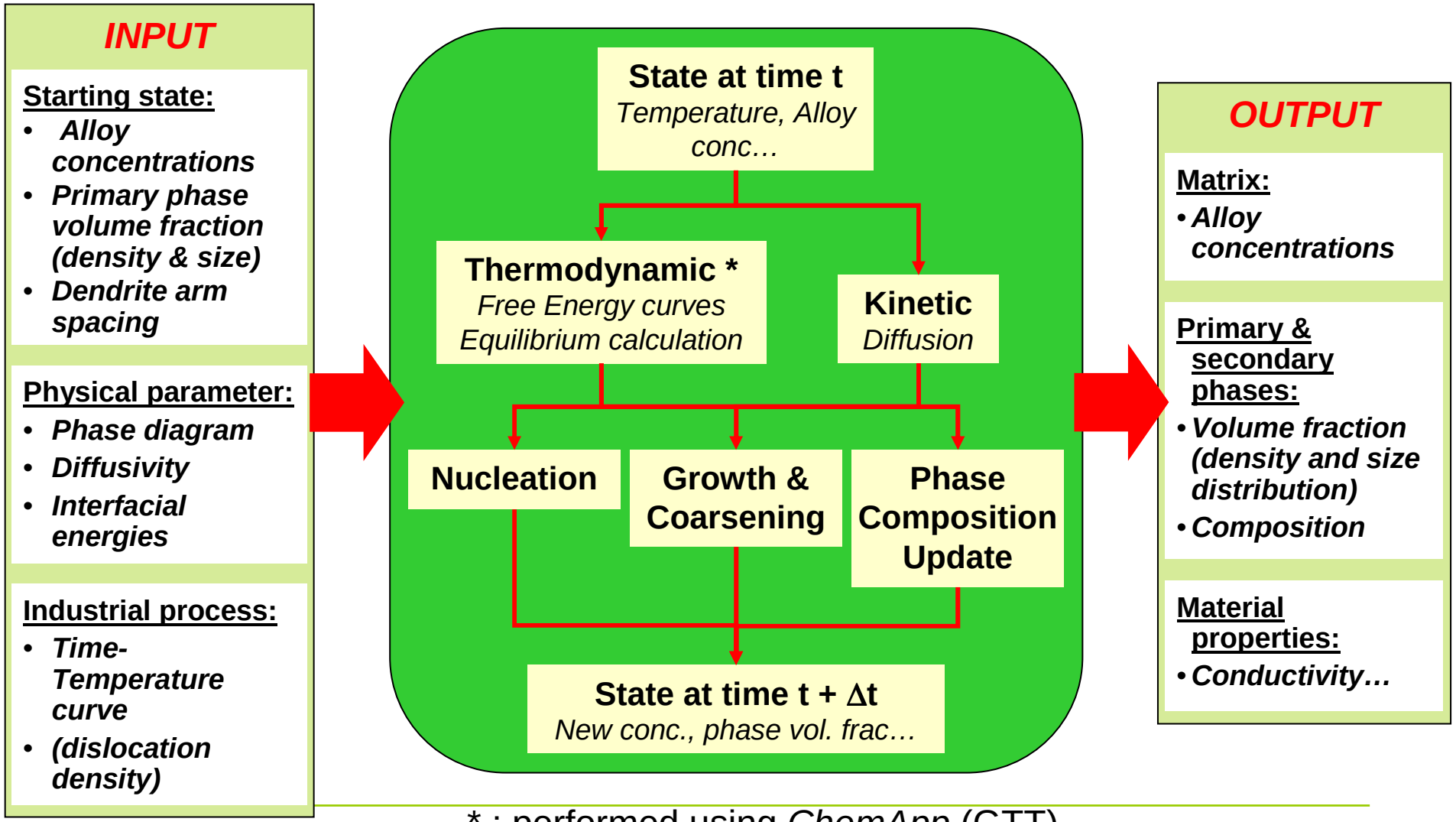
ClaNG model overview



* : performed using *ChemApp* (GTT)

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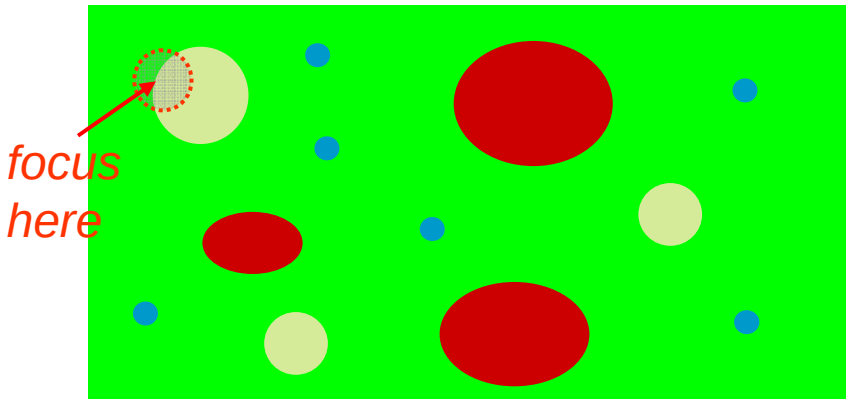
Thermodynamic calculations (I)

At every interface, one assumes that a local equilibrium is achieved after a short time



For each possible phase (*Mg_2Si, alpha,* …) perform the chemical reaction corresponding to the matrix decomposition occurring at the interface between the matrix and the phase

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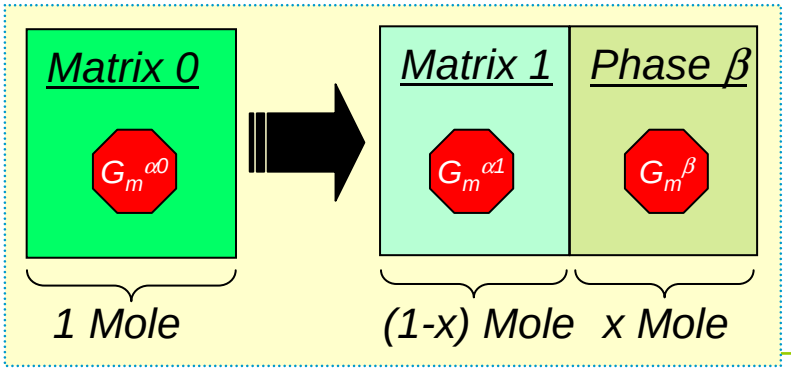
Thermodynamic calculations (II)

Use of ChemApp:

- Set initial conditions (temperature, concentrations in the matrix)
- Enter two phases: matrix + another phase
- Perform equilibrium
- Extract necessary information
  - equilibrium concentrations c_i^{α} in the Al matrix α
  - equilibrium concentrations c_i^{β} in the phase β
  - chemical potentials of the elements
- Derive the Chemical Driving Force Δg_u



$$\Delta g_u^{\beta} = \sum_i c_i^{\beta} \cdot (\mu_i^{\alpha 0} - \mu_i^{\alpha 1})$$

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ClaNG / Nucleation

When Δg_u is known, the critical radius r_c can be derived

$$r_c = \frac{2\gamma \cdot V_m}{\Delta g_u}$$

γ: interfacial energy (model input)

The nucleation rate is then given by the classical theory of Becker & Döring

$$\dot{N} = N_0 \cdot Z \cdot \beta \cdot \exp\left(-f_{het} \cdot \frac{\Delta G(r_C)}{k_B \cdot T}\right) \cdot \exp\left(\frac{-\tau}{t}\right)$$

Z: (Zeldovich factor) normalization variable describing the dissolution of nuclei

β: rate at which solute atoms join the critical radius

$\Delta G(r_c)$: Gibbs energy for a spherical nucleus

k_B: Boltzmann constant

f_{het}: scaling factor for heterogeneous nucleation (0.1 … 1.0)

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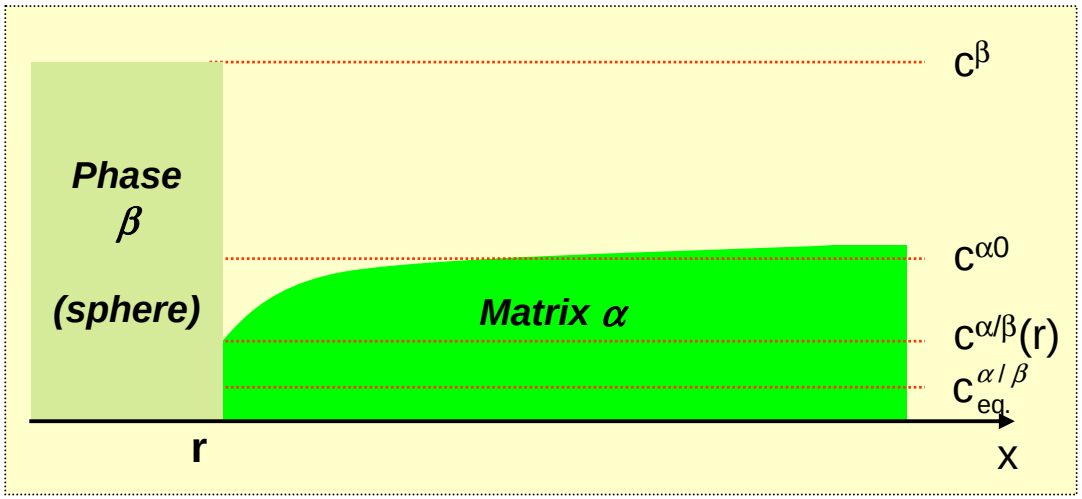
ClaNG/ Growth & Coarsening

Assumption: precipitate growth diffusion controlled in Al alloys

ClaNG treats growth and coarsening in a single equation

- A particle above the critical radius grows
- A particle below the critical radius dissolves

The growth law used in ClaNG derives from Zener's formulation (spherical particles)



$$v = \frac{dr}{dt} = \frac{c^{\alpha 0} - c^{\alpha/\beta}(r)}{c^{\beta} - c^{\alpha/\beta}(r)} \cdot \frac{D}{r}$$

$$c^{\alpha/\beta}(r) = c_{eq}^{\alpha/\beta} \cdot \exp\left(\frac{2\gamma \cdot V_m}{R_g T \cdot r}\right)$$

Gibbs-Thomson concentration at the interface

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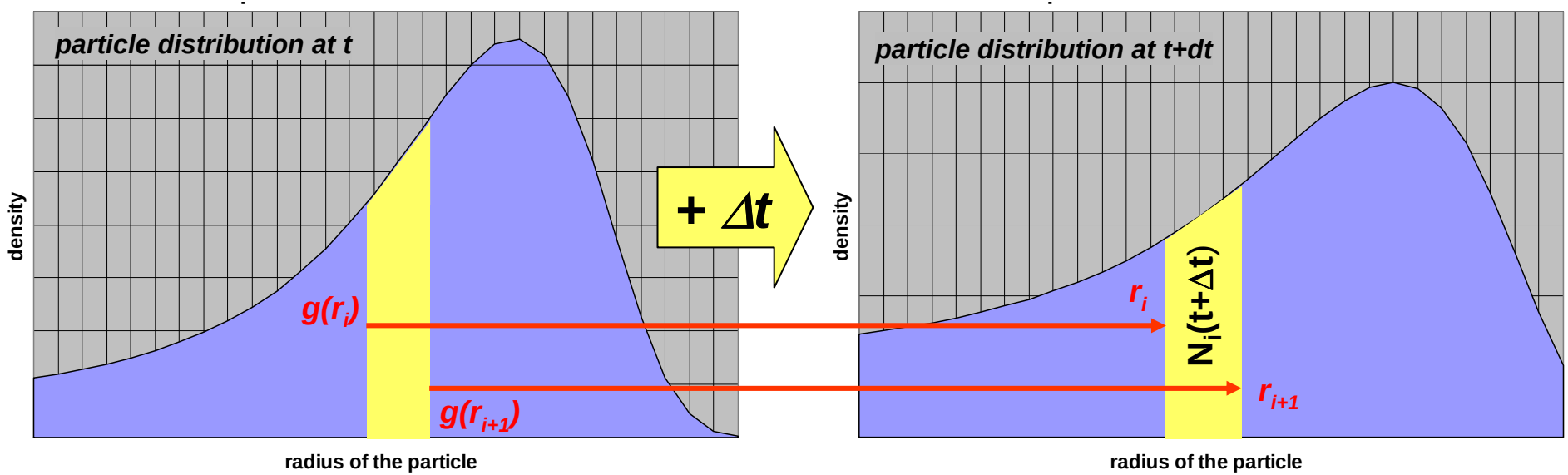
Evolution with time

evolution of the whole number and size distribution *f(r,t)* by combining the nucleation rate and the growth law in the continuity equation (discretization in radius classes, e.g. 1 nm)



For every radius r_i at $t+\Delta t$, one determines its image $g(r_i)$ at t using a Runge-Kutta method

$$N_i(t+\Delta t) = N_i(t) + \int_{g(r_i)}^{r_i} f(r,t)\cdot dr - \int_{g(r_{i+1})}^{r_{i+1}} f(r,t)\cdot dr \qquad \left(+ \dot{N}_i^{nucl}\,\Delta t\right)$$

(Robson, Acta Mater. 51, 2003)

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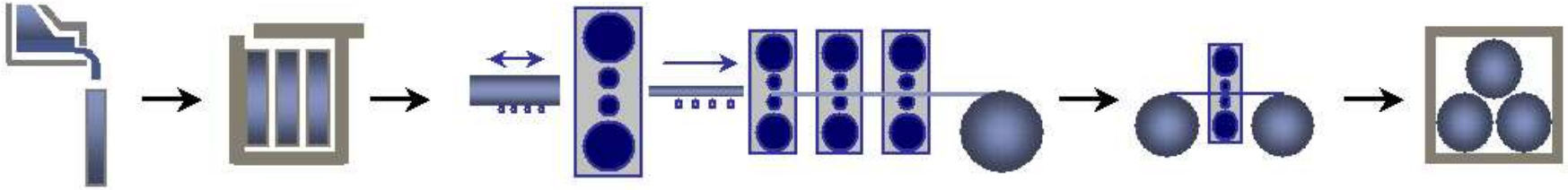
ClaNG Modell
"*Cla*ssical *N*ucleation and *G*rowth"



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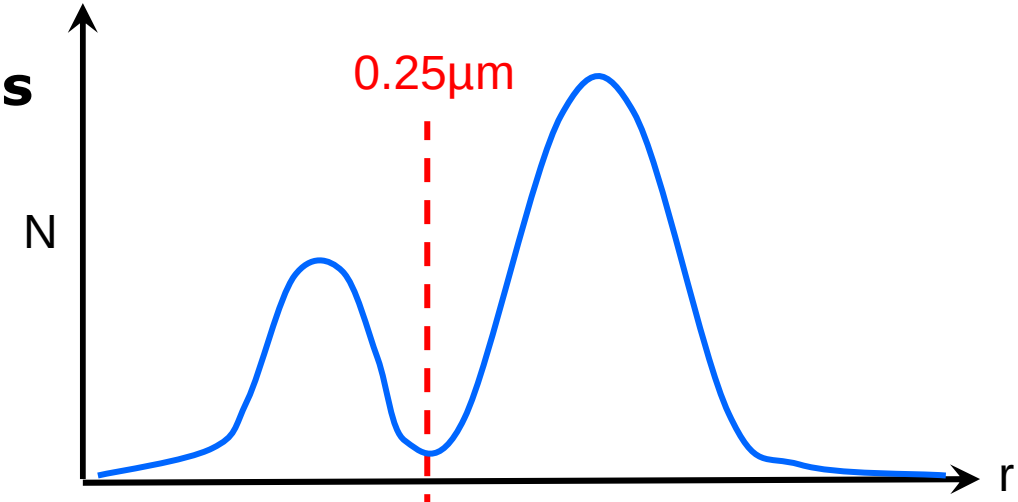
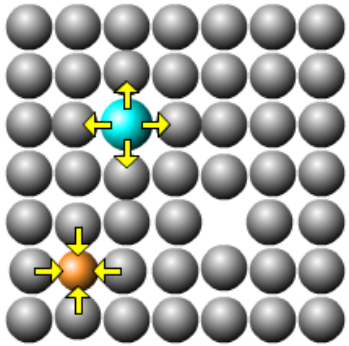
Micro-chemistry
- solute levels c_i
- particles $V_i(r)$
- type, size, volume

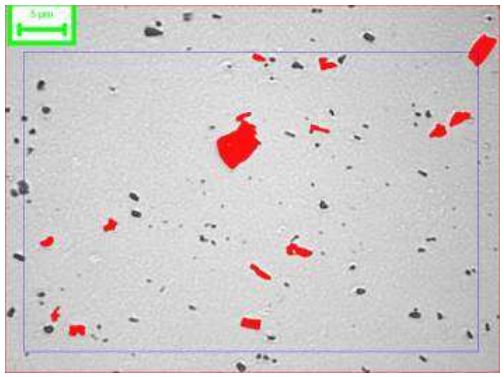
Input → ClaNG-Model → Output

Microchemistry microstructural features

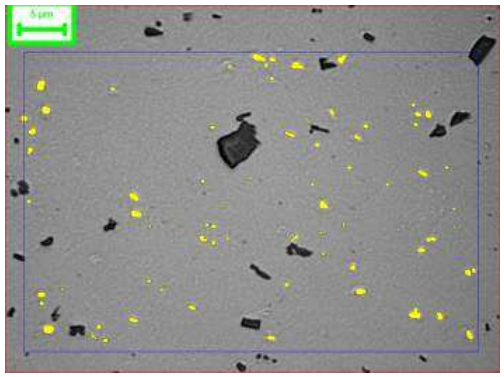




solute atoms



dispersoids / secondary phases
(precipitation in solid state
0.01-0.1µm)



constituents
(as-cast
1…20µm)

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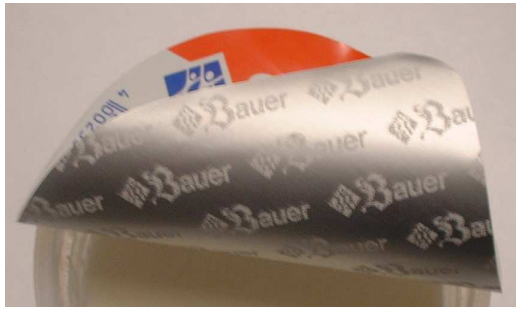
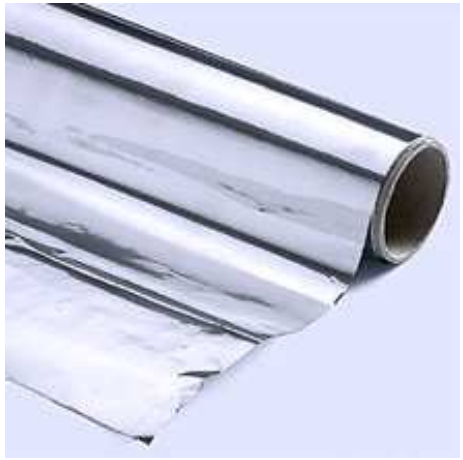
Use of Al foil

thickness range 6 … 200 µm

Use

- industrial applications (heat exchanger, cable mantling, electronics, …)
- packaging applications





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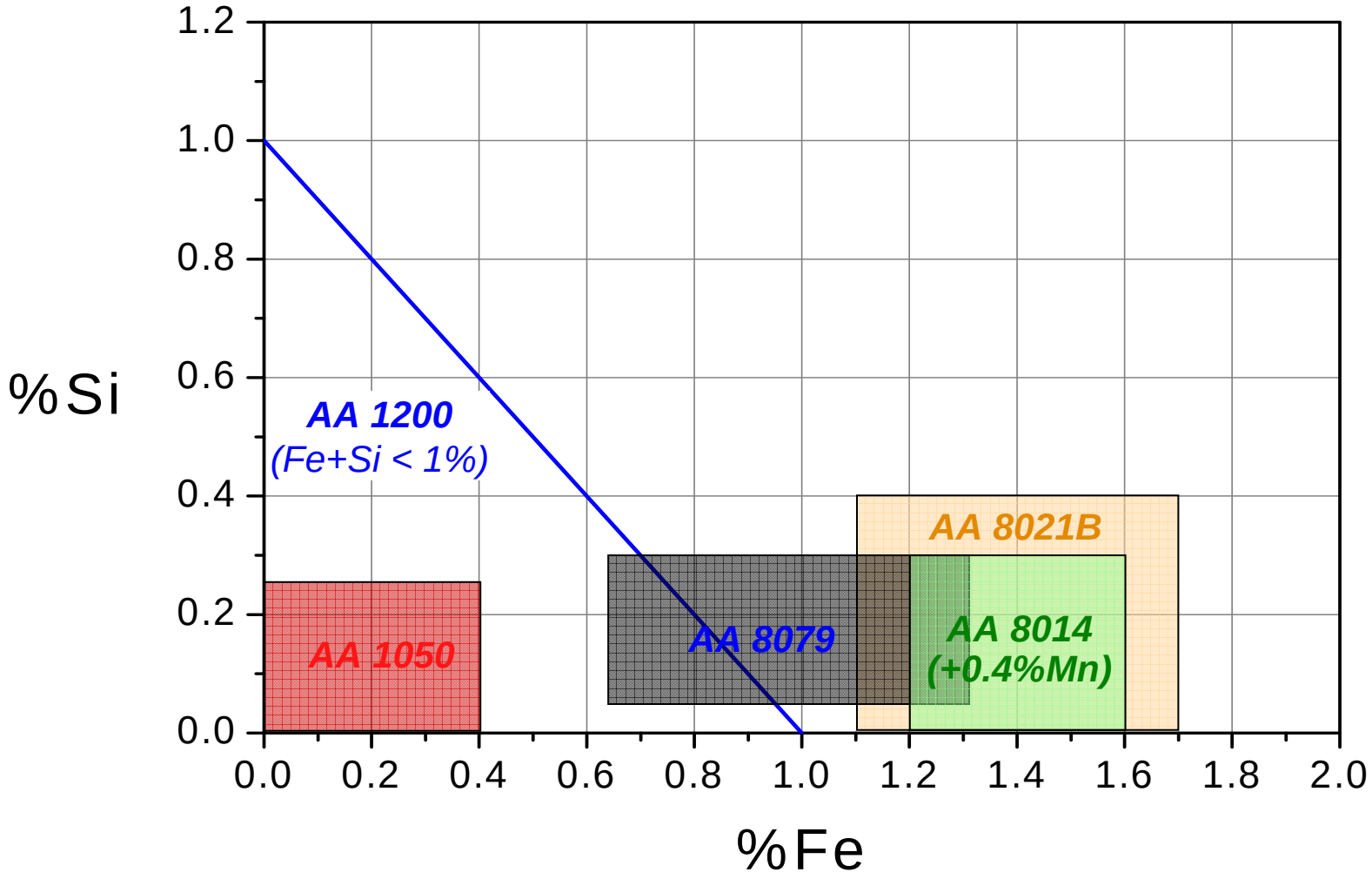
Composition of most important foil alloys
1xxx, 8xxx



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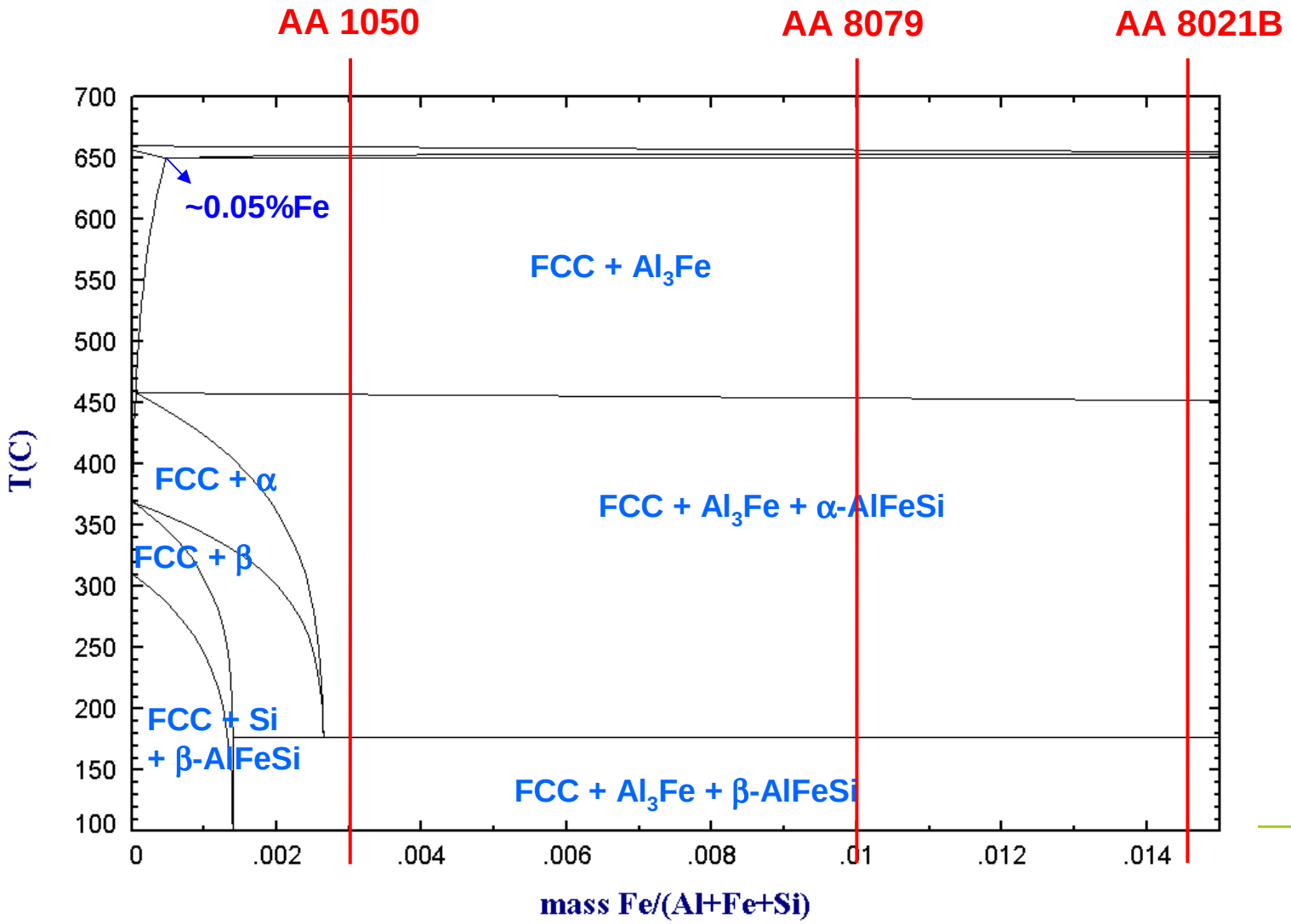
Al-Fe-Si phase diagram (0.07%Si)
FactSage (database AlTT15)



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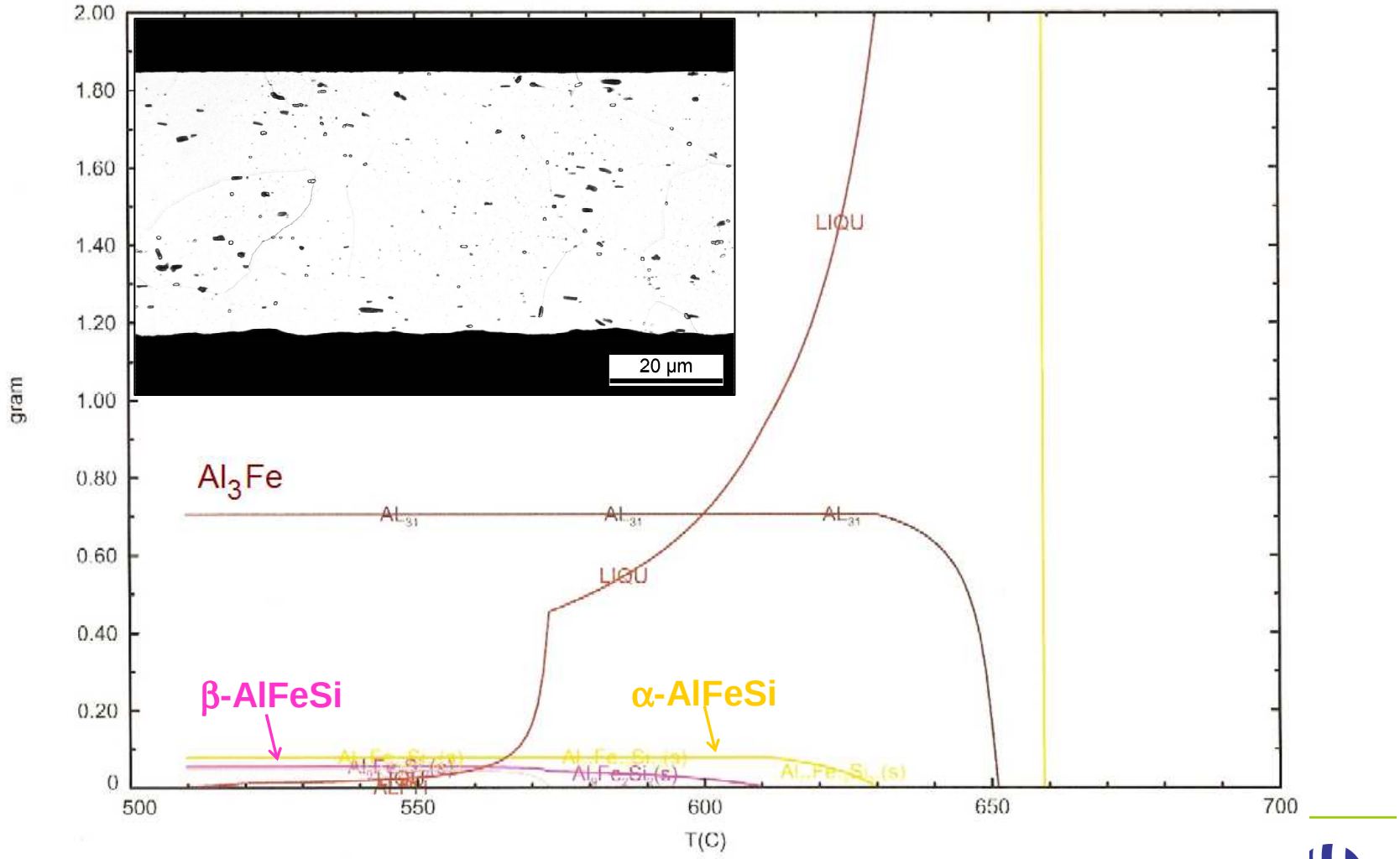
HA 1200-N, Scheil-Diagram FactSage (database AlTT15)



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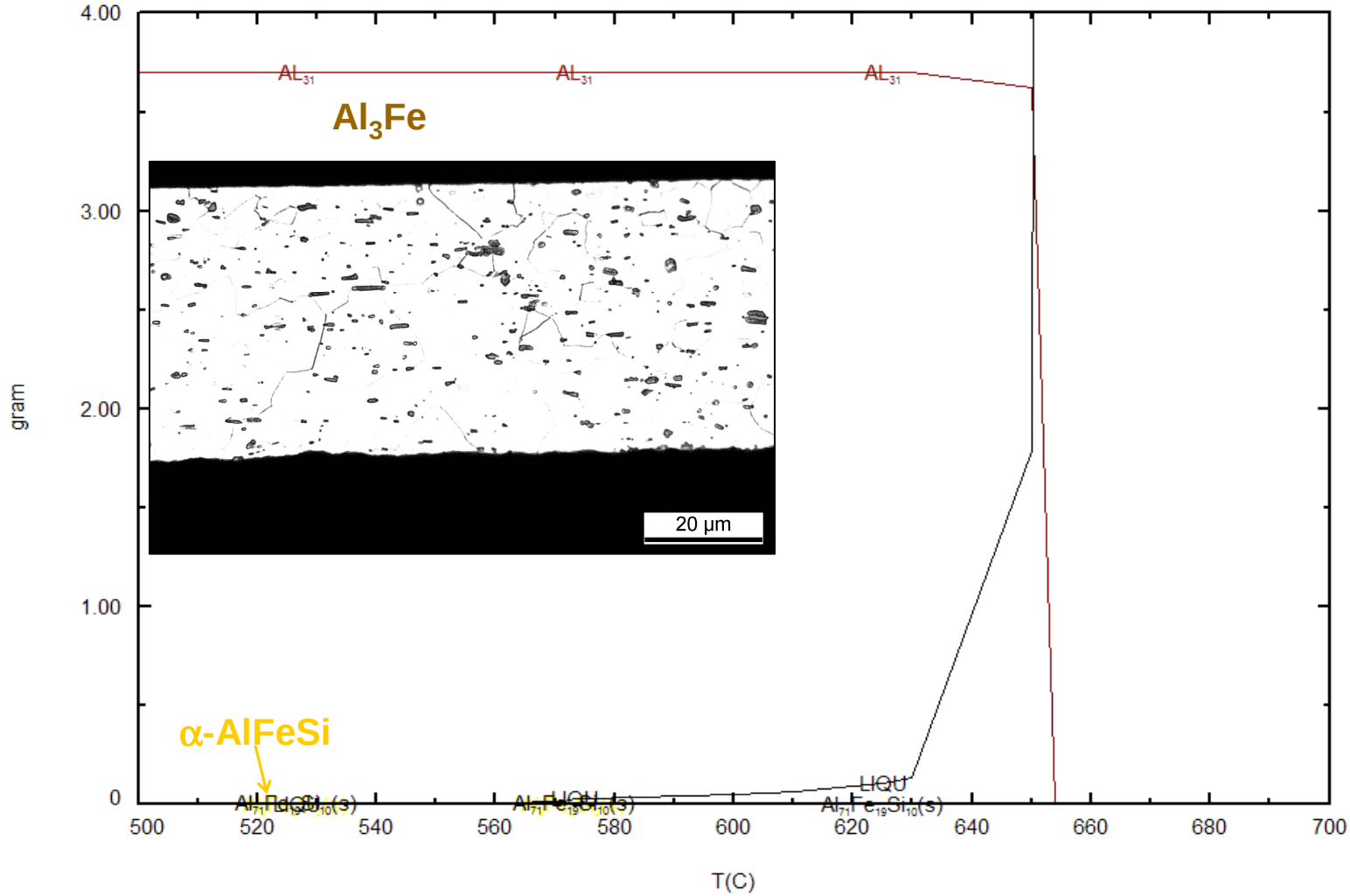
HA 8021-F, Scheil-Diagram FactSage (database AlTT15)



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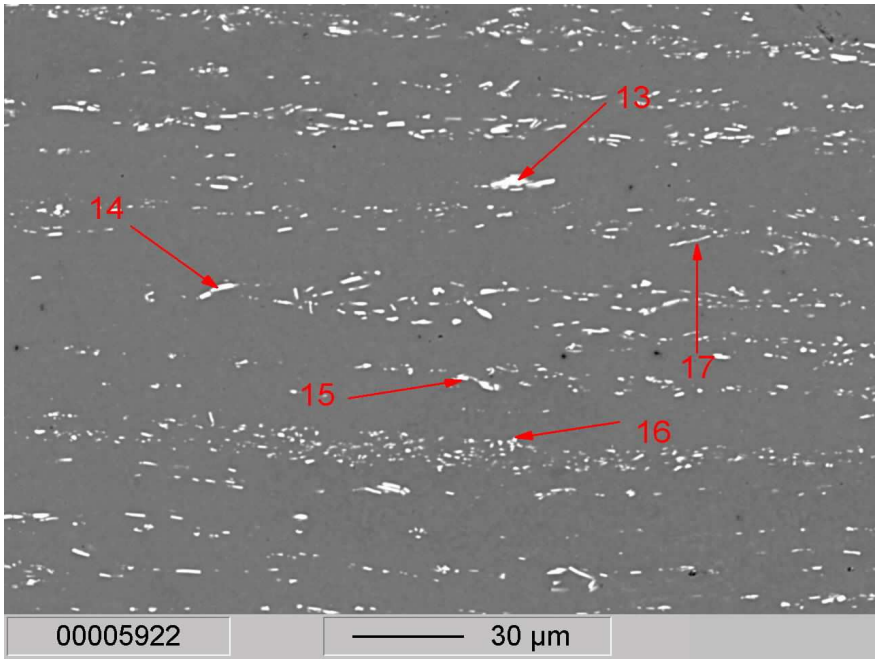
Experimental validation: microprobe investigations in 8xxx transfer gauge material



Pos.	Si	Mn	Fe	Rest Al
wie 1	0,5	0,1	35,6	
wie 5	0,5	0,1	32,5	
wie 8	0,5	0,1	31,6	
wie 13	0,4	0,1	30,9	
wie 14	0,3	0,1	30,3	
außerhalb Bild *	0,4	0,1	30,0	

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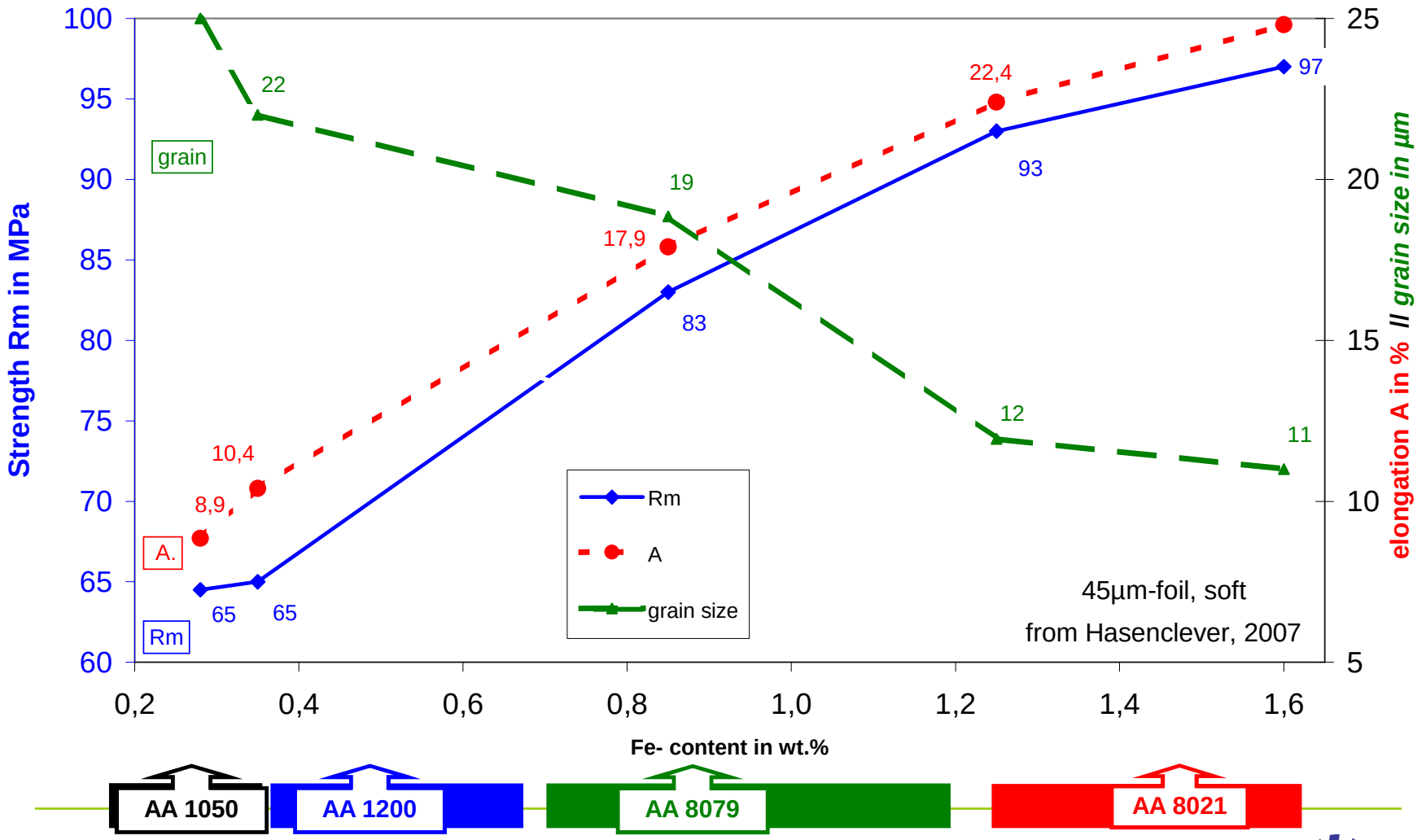
Mechanical properties of most important foil alloys (soft)



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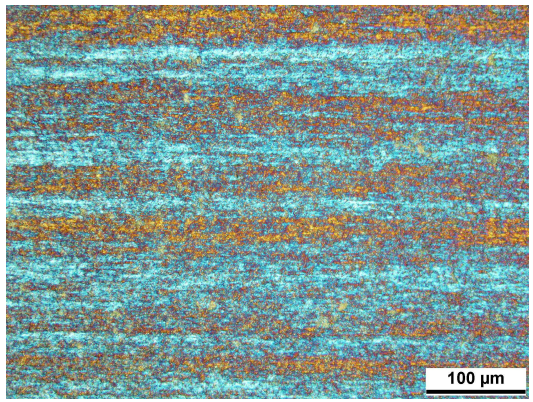
Impact of final annealing on microstructure and properties of Al foil

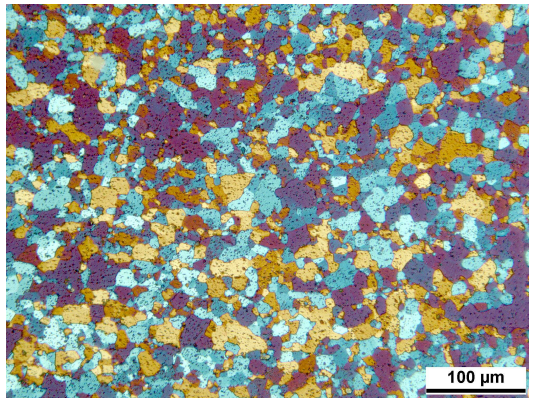
not annealed (hard)

R_p = 140 - 170 MPa
A_{100mm} = 1 … 4%



soft annealed

R_p= 30 - 60 MPa
A_{100mm} = 20 … 30%



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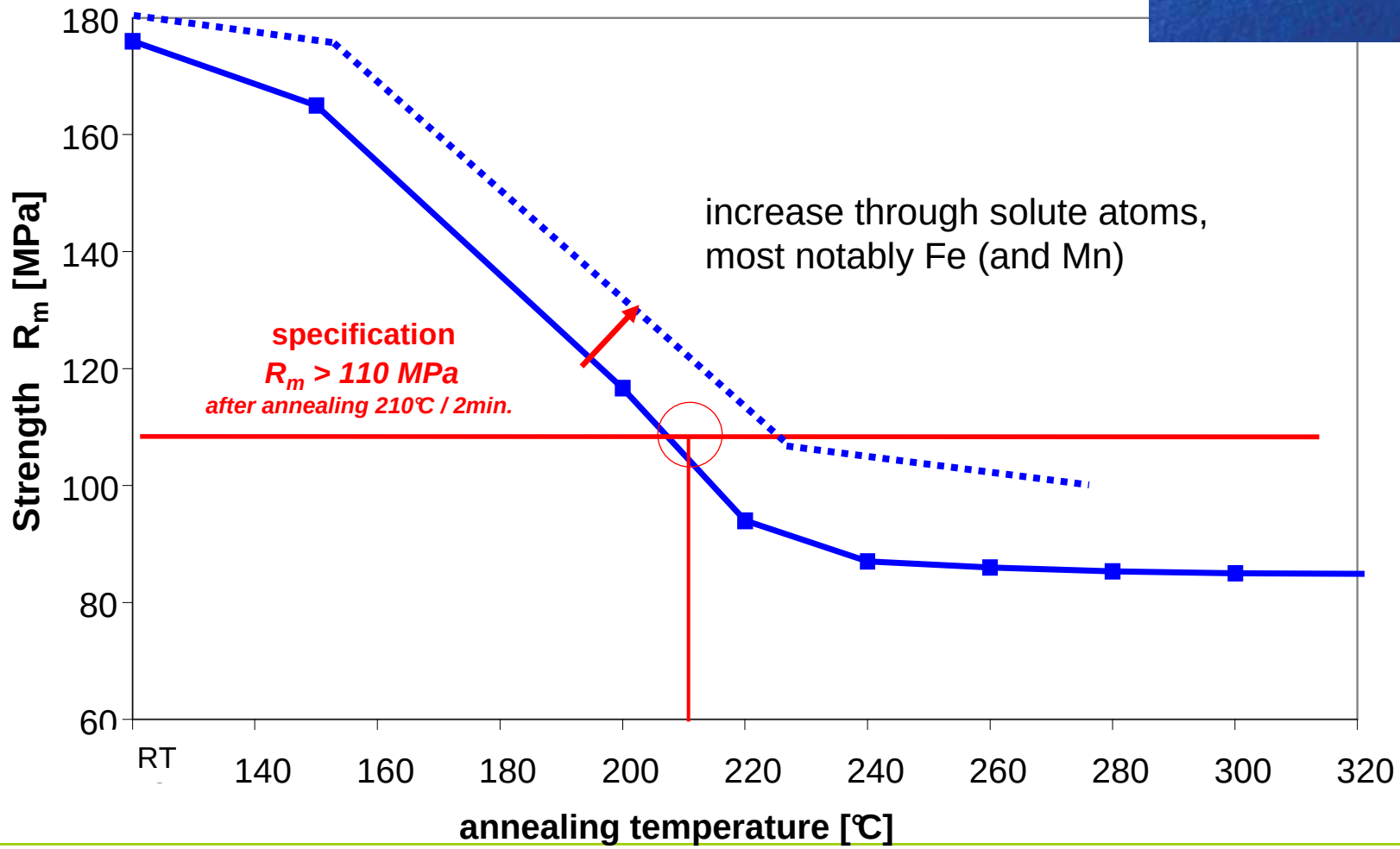
Thermal stability of Al blister foil



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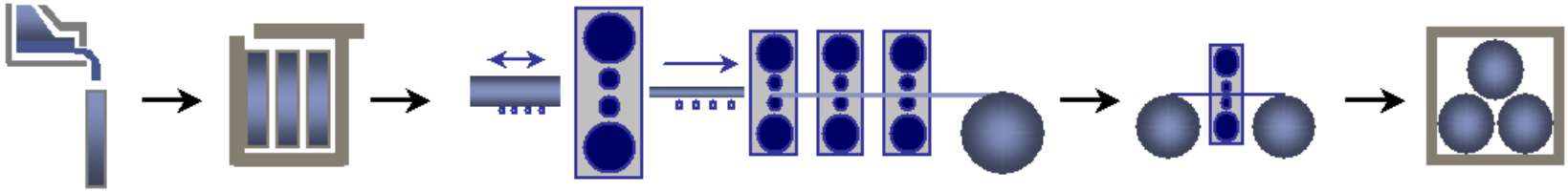

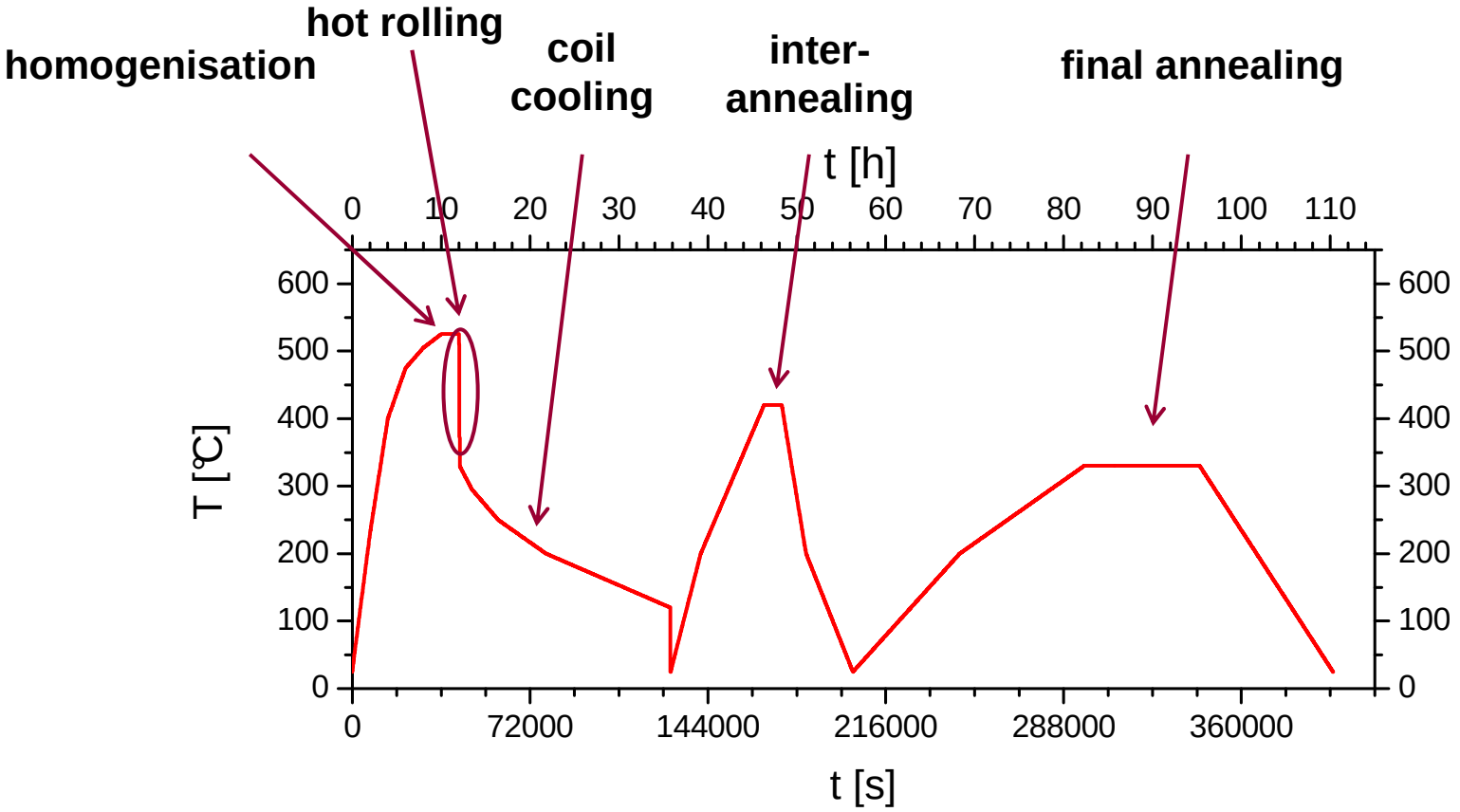

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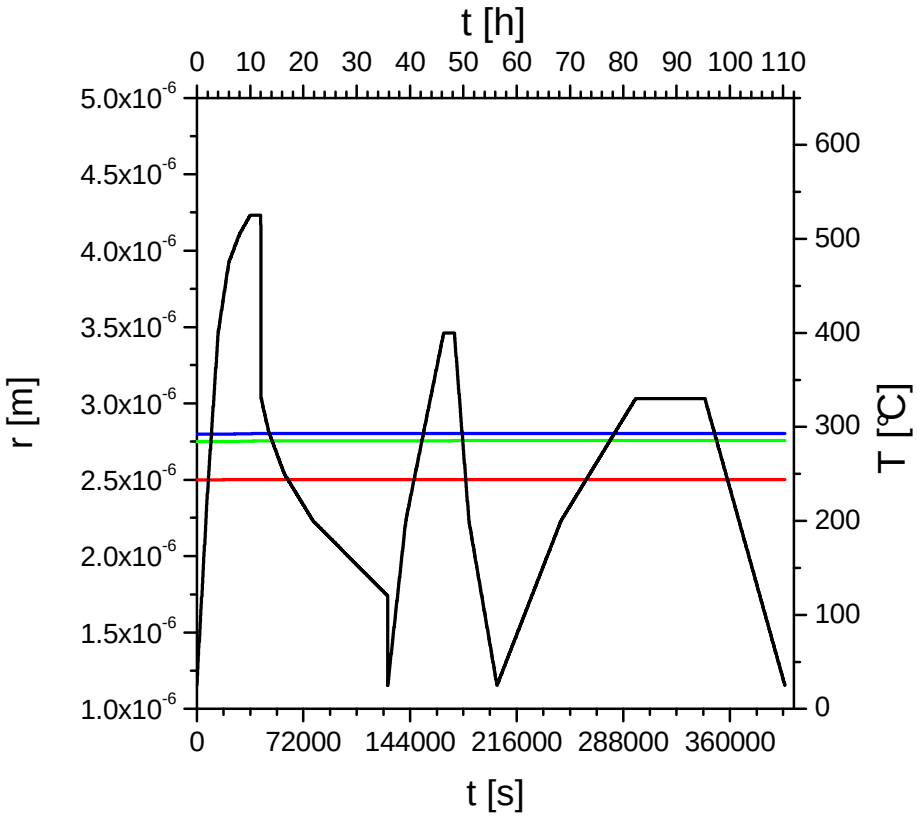
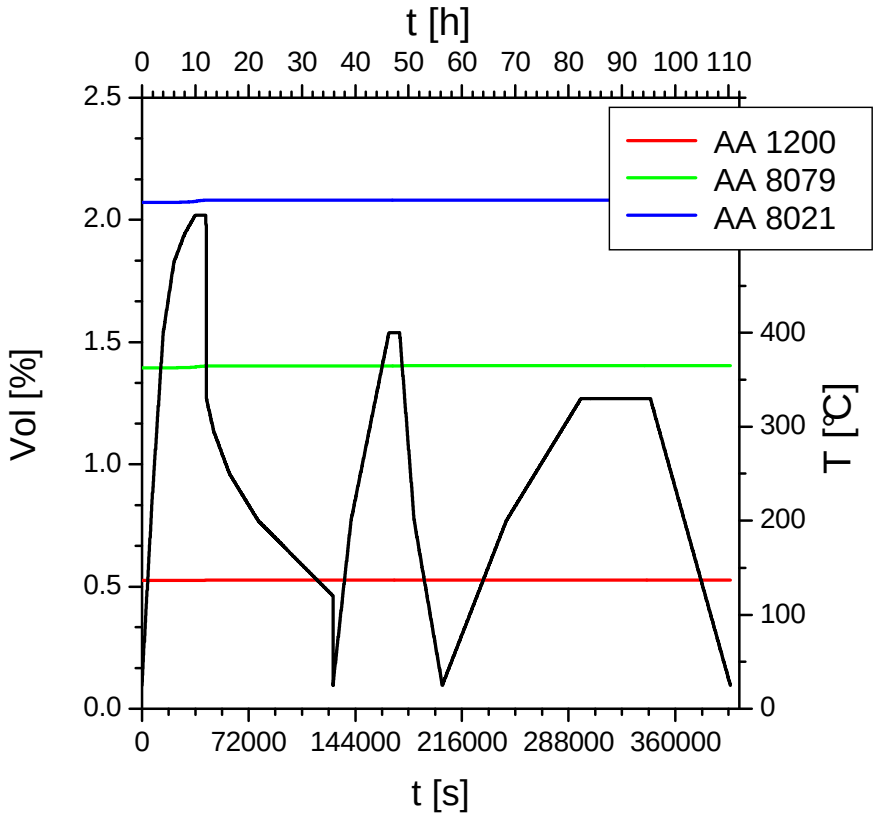
ClaNG results / large particles
Al_3Fe-constituents (>0.25µm)





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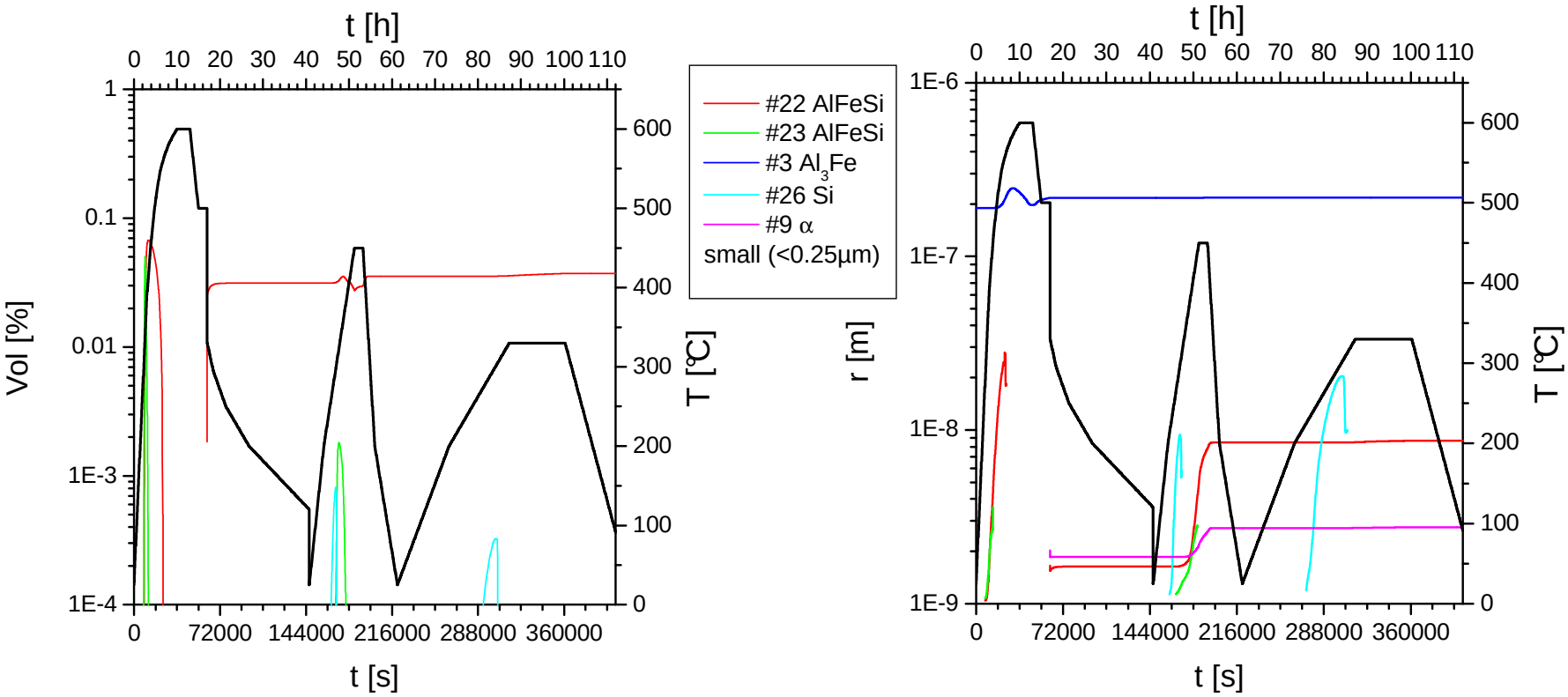
ClaNG results / small dispersoids (<0.25µm)



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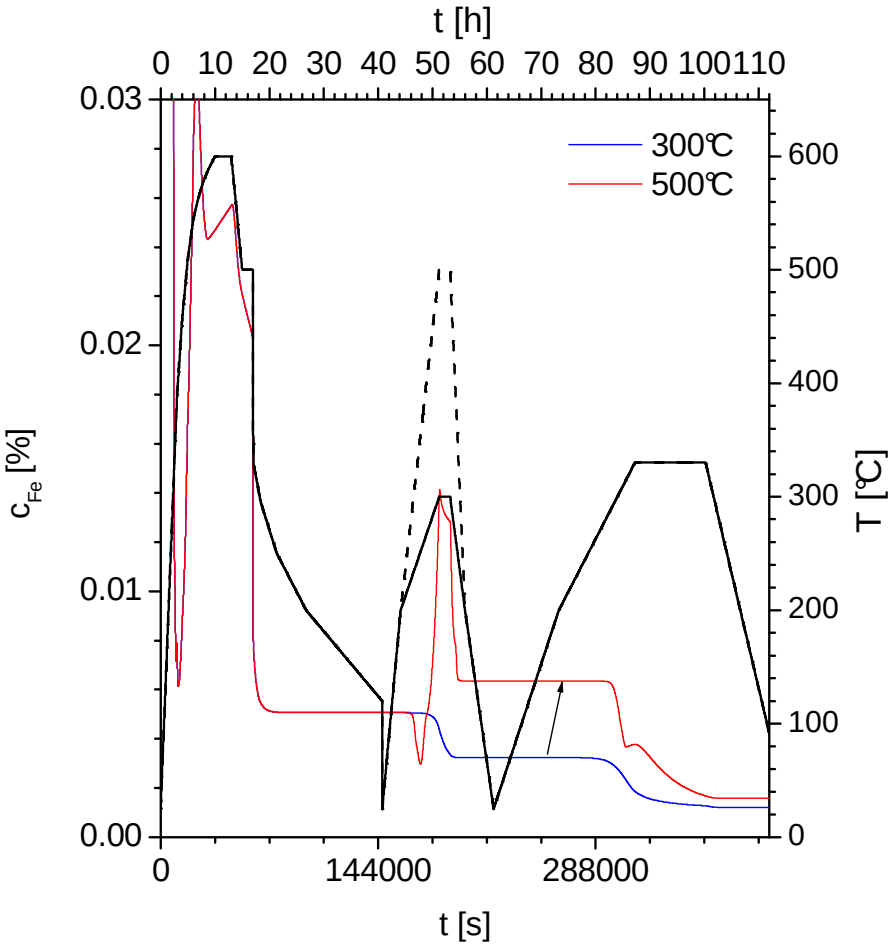
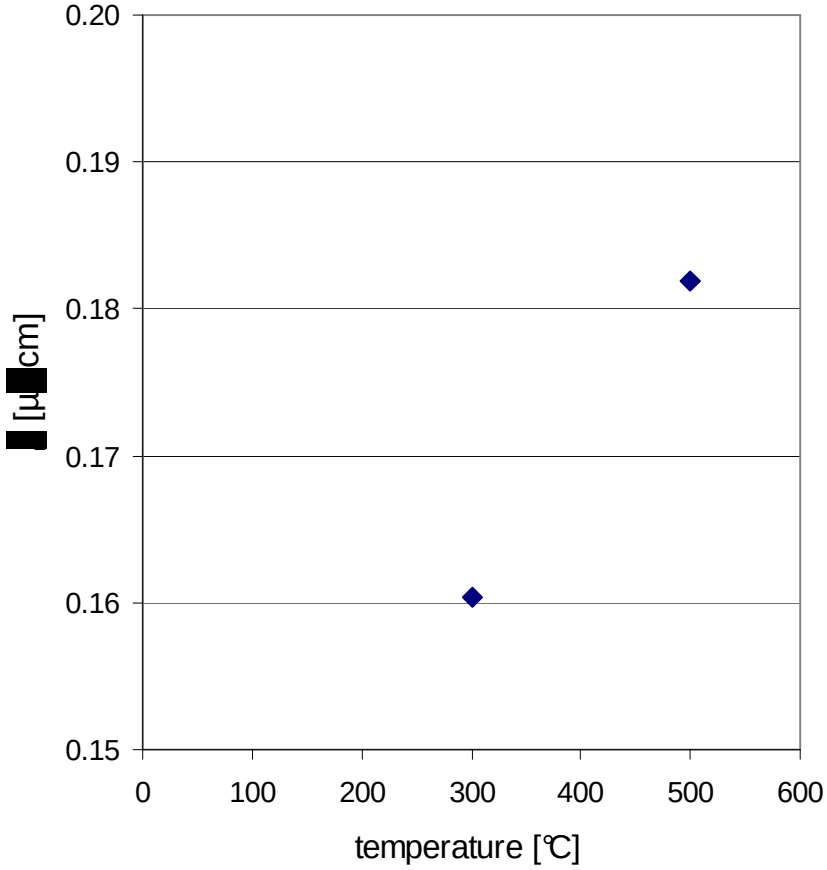
Impact of inter-annealing temperature on solute Fe





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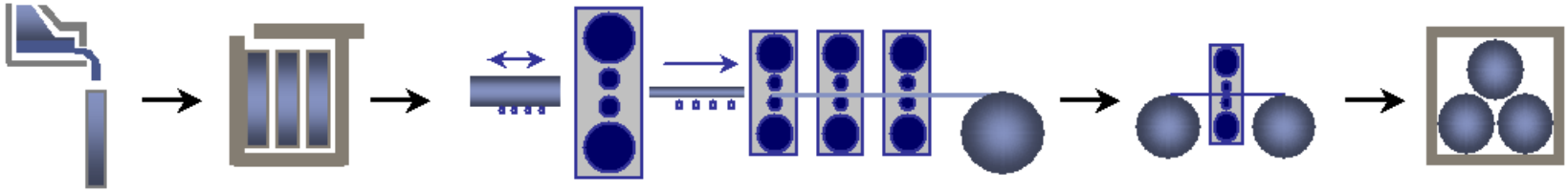
Summary and Conclusions



Through-process modeling: coupling of models for simulating the evolution of

- deformation
- softening (recovery and recrystallization)
- **micro-chemistry**
- properties

The ClaNG model (ChemApp) allows analysing the evolution of micro-chemistry (solutes, particles) along the process chain

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