Global and local equilibrium during solidification - modelling of microsegregation

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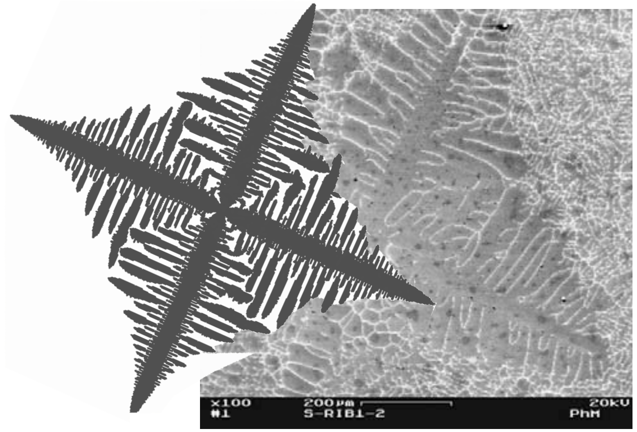
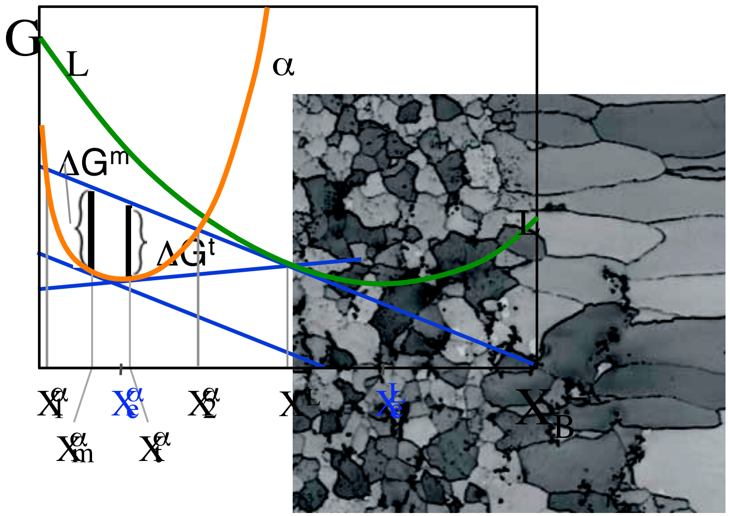
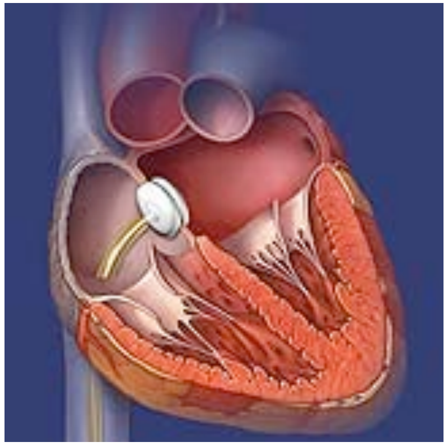
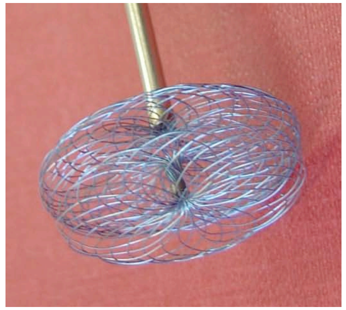
research fields



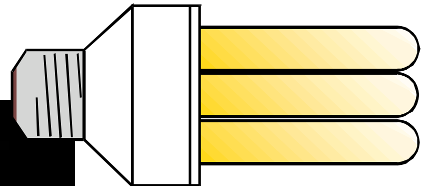
structure formation
(non-equilibrium) thermodynamics





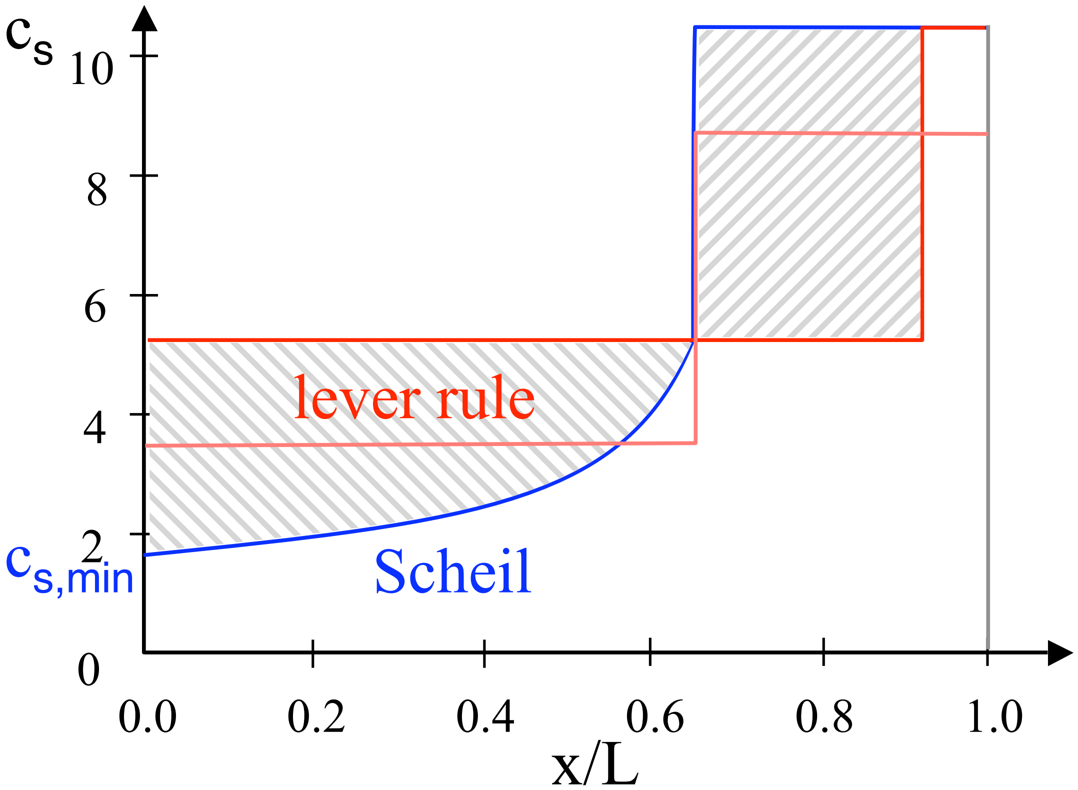


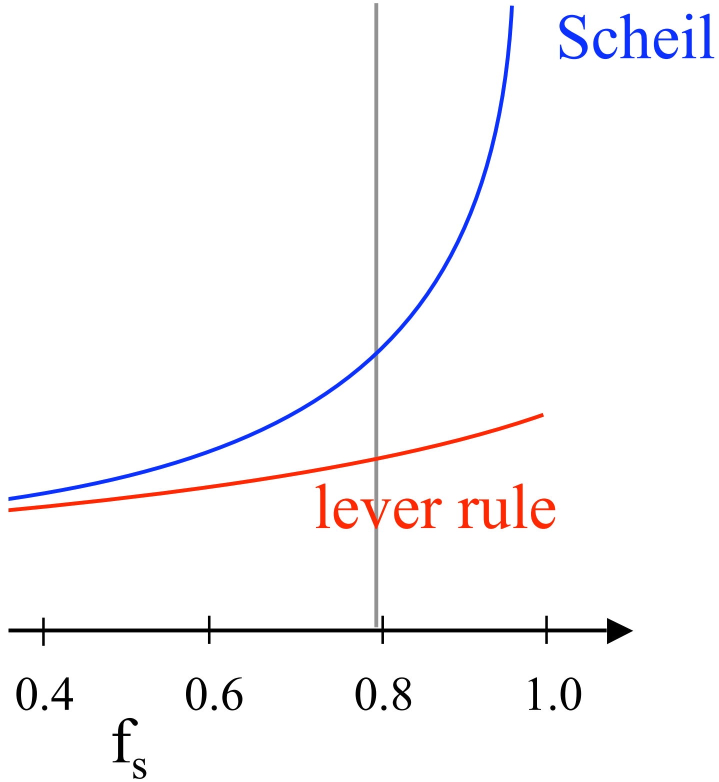
implant alloys



alloy development

global equilibrium and Scheil





Scheil:

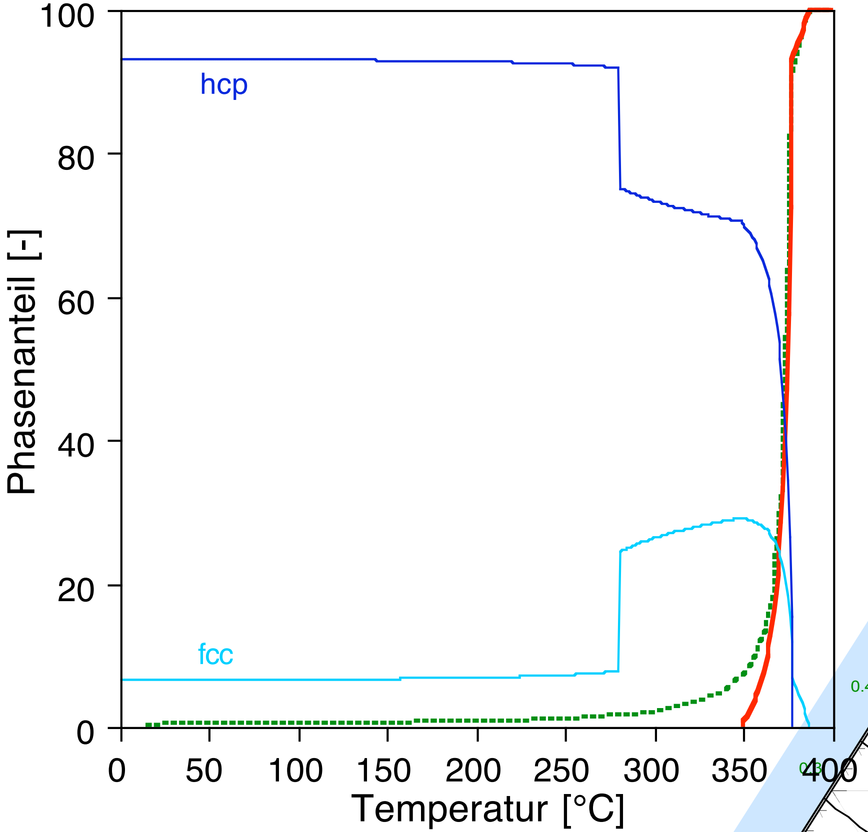
- starts at $c_{s,min} = k_{eq} \cdot c_0$
- ends at $c_{s,max} = \infty$ ($\Rightarrow$ divergent)

Scheil: $c^*(t)$ <u>and</u> $c(x)$

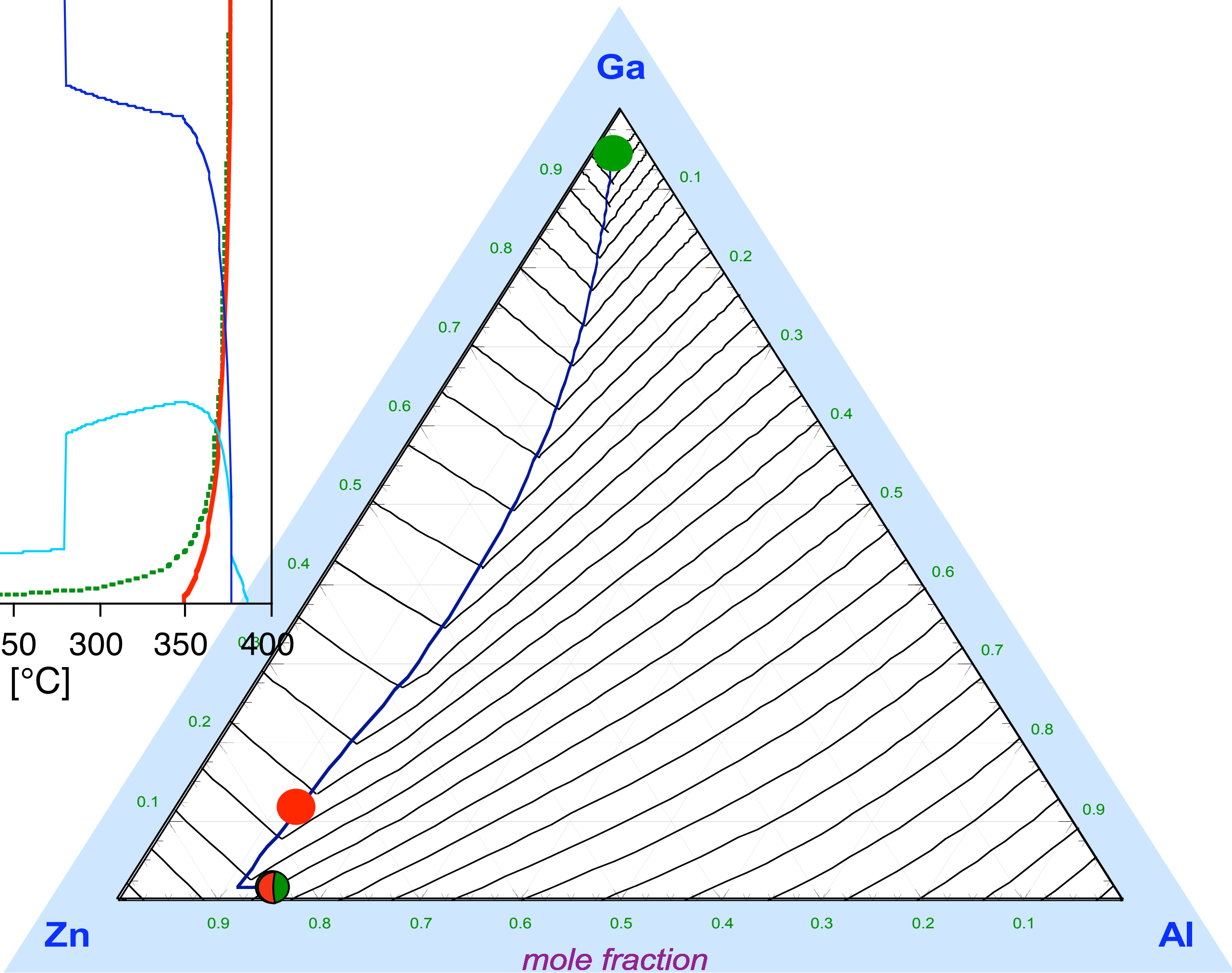
lever rule: $c^*(t)$

example: Al-Zn-Ga solder

- lever rule
- Scheil

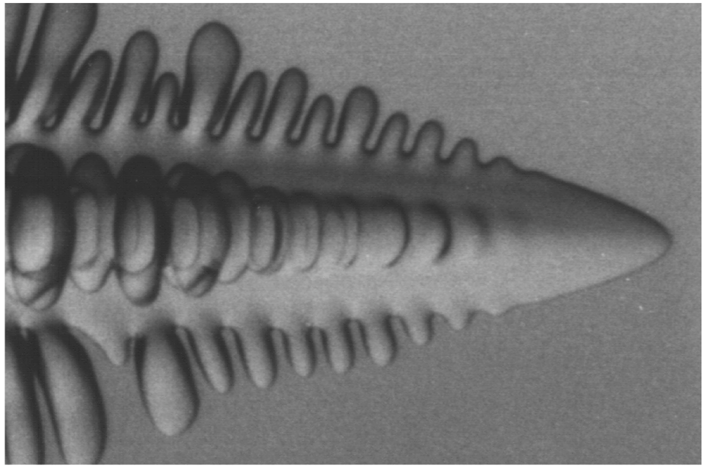


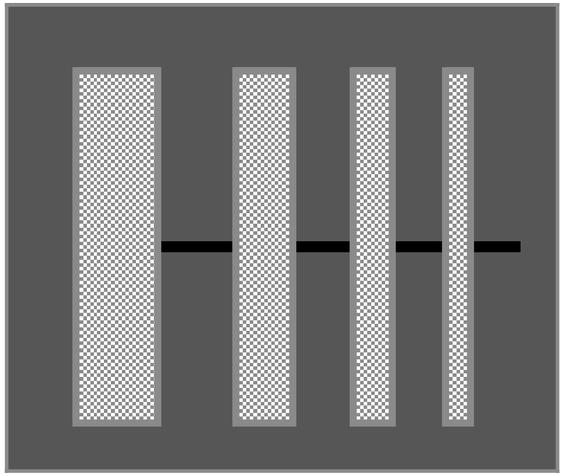
liquid Ga-rich phase
at room temperature

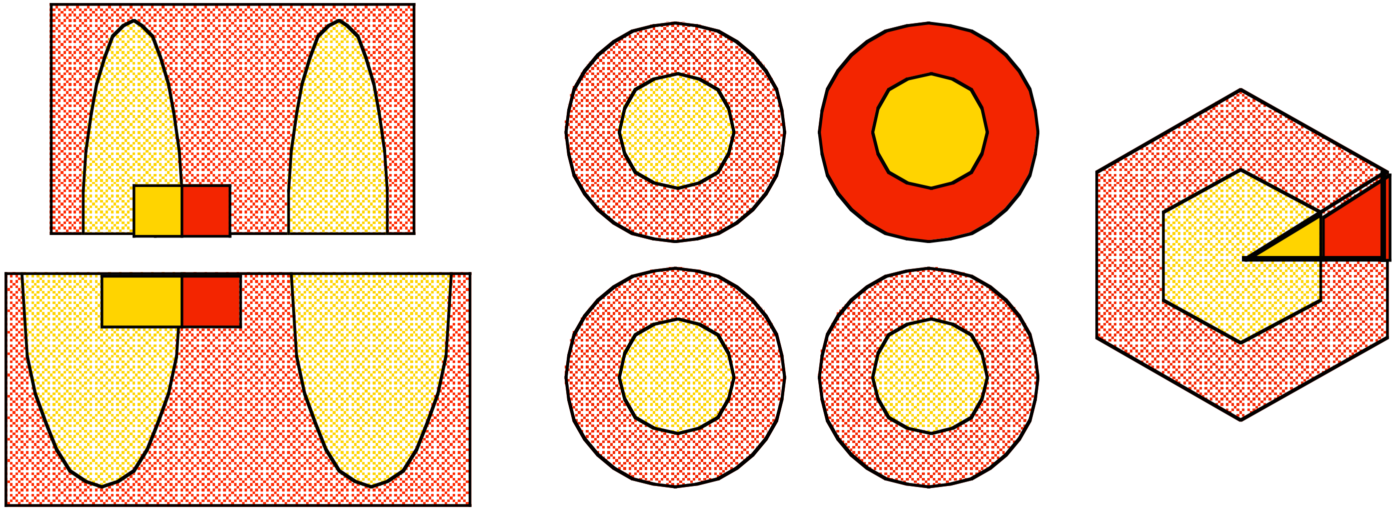


geometry in micromodels

'plate model'

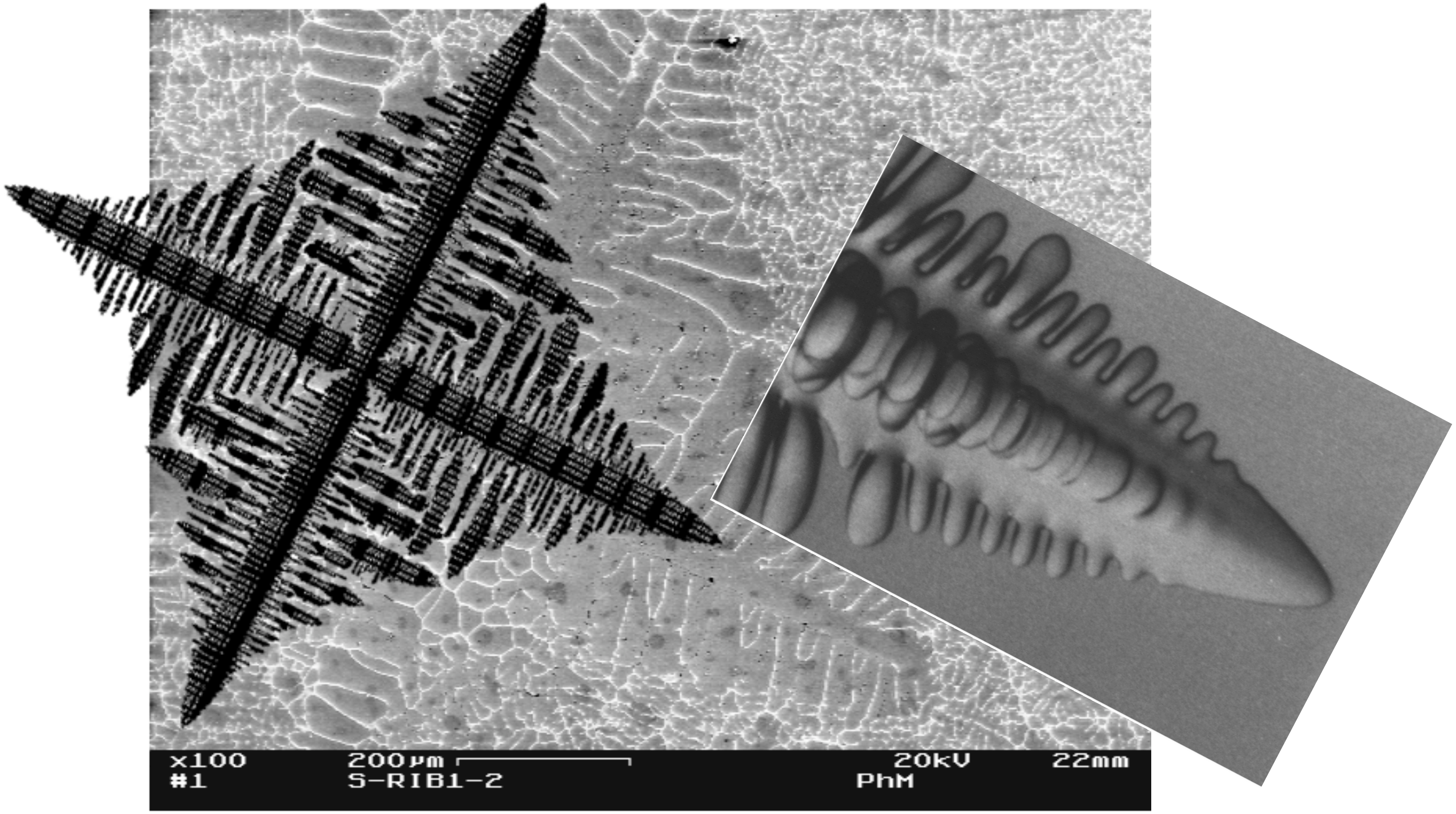






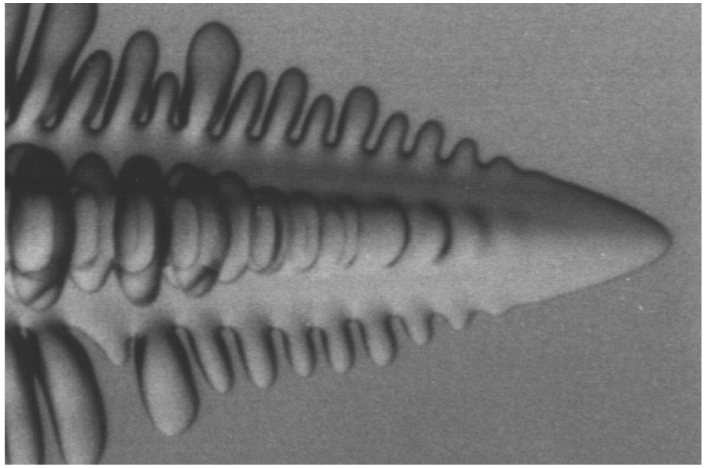
symmetry elements

2D model?

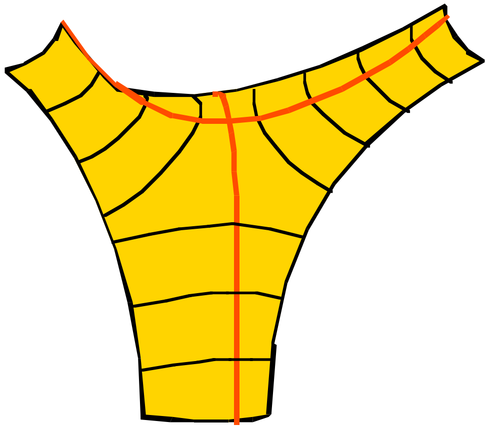


2D models tend to overestimate the local solid fraction

curvature

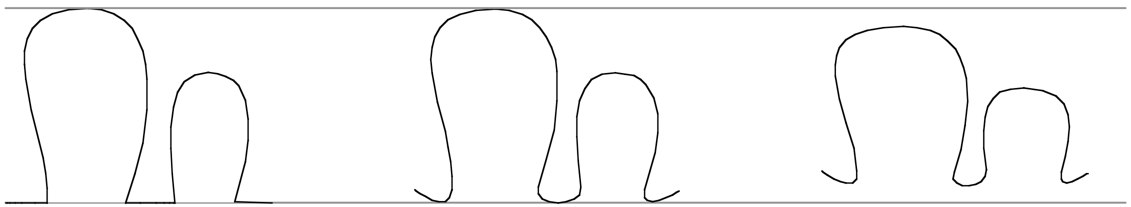


experimental observations:
- tip of secondary arm is thicker than root
- equilibration occurs at root



$$K = \frac{1}{r_1} + \frac{1}{r_2}$$

$\Rightarrow$ saddle points

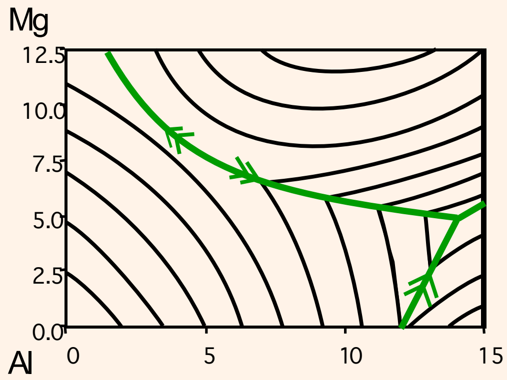


2D coarsening?

$\Rightarrow$ curvature in 2D is qualitatively wrong!

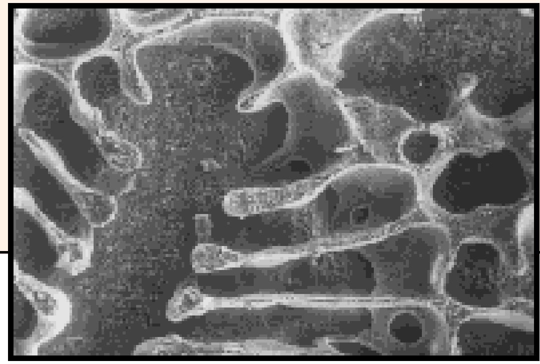
effects of curvature in 1D can be considered statistically

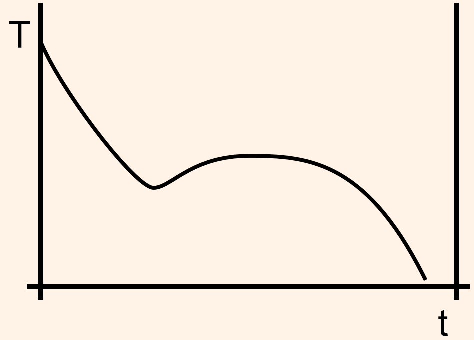
extended 1D-model



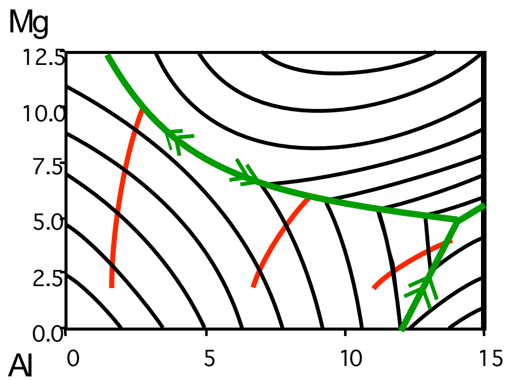
phase diagram
(tie lines)

$D_s(T)$, $D_\ell(T)$	diffusion
σ, ΔS_f	coarsening
σ, ΔS_f	grwoth undercoolings
ϕi	ΔT_E
...	...

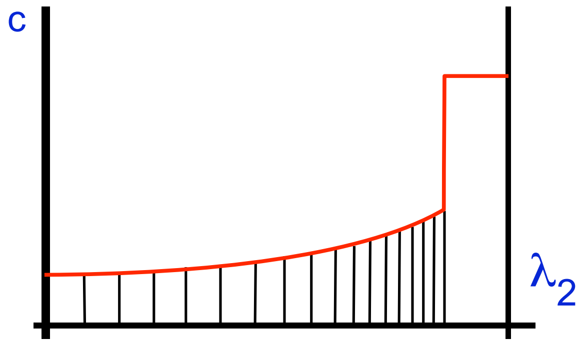




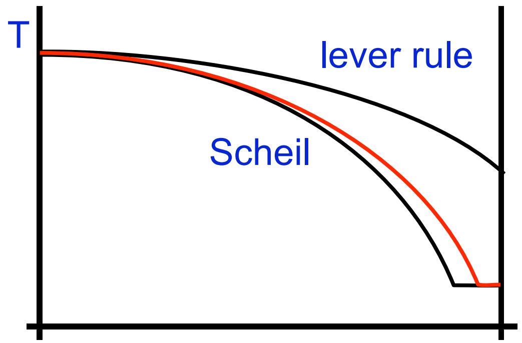
cooling curve



solidification path



concentration profile
phase fractions

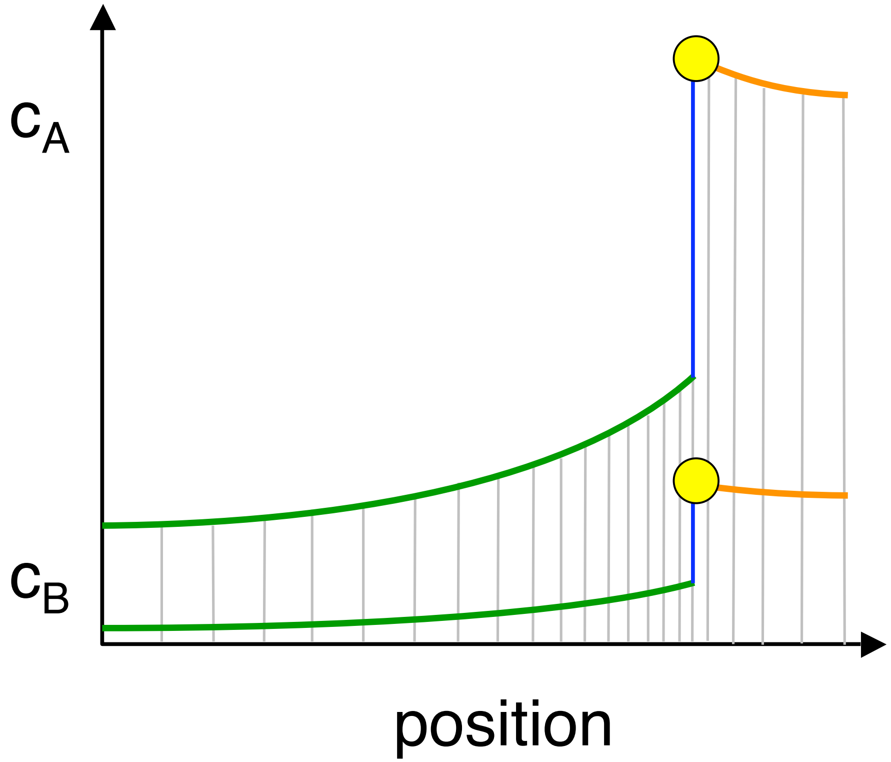


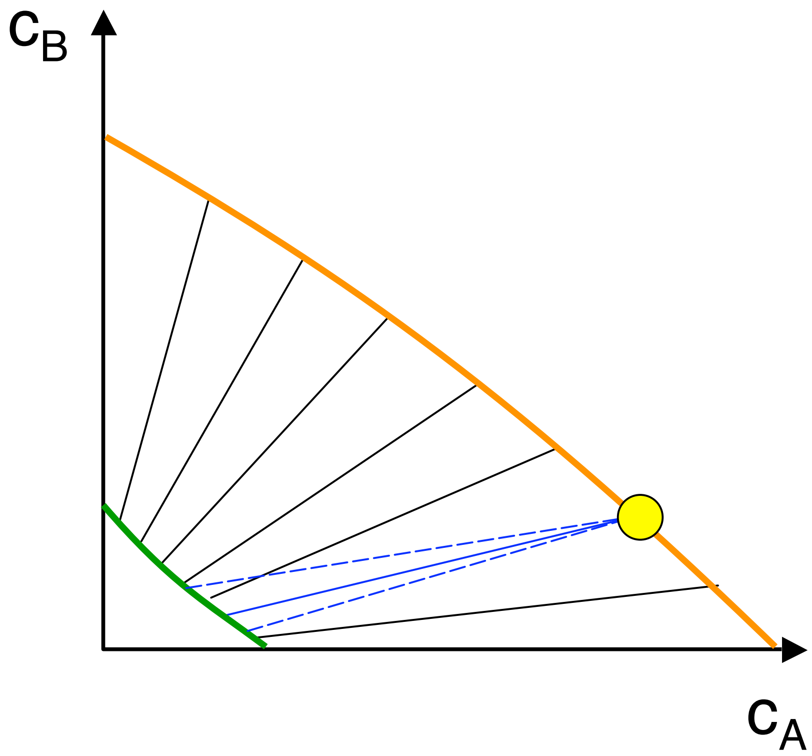
solid fraction
solidification temperature

coupling with phase diagram

- evolution of concentration profile diffusion controlled
- interface concentrations connected through phase diagram

empirical phase diagram:
tie-lines not defined
⇒ calculate tie-lines with ChemApp



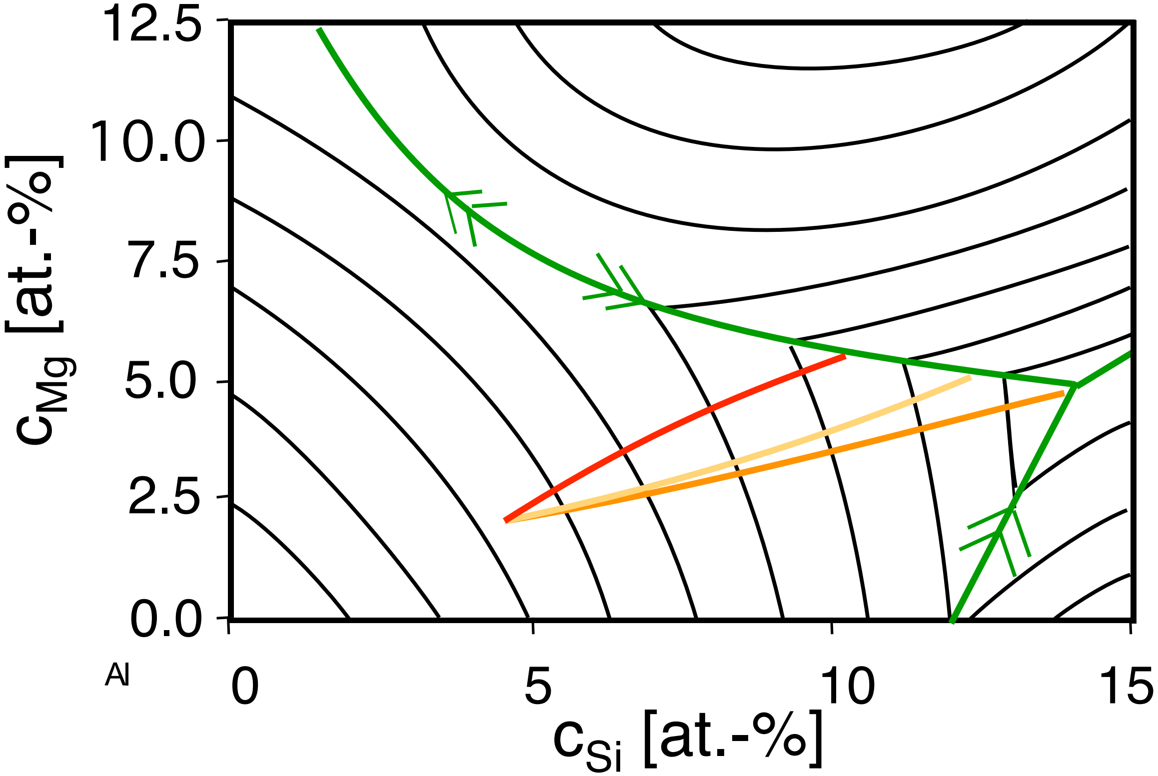


solidification paths:

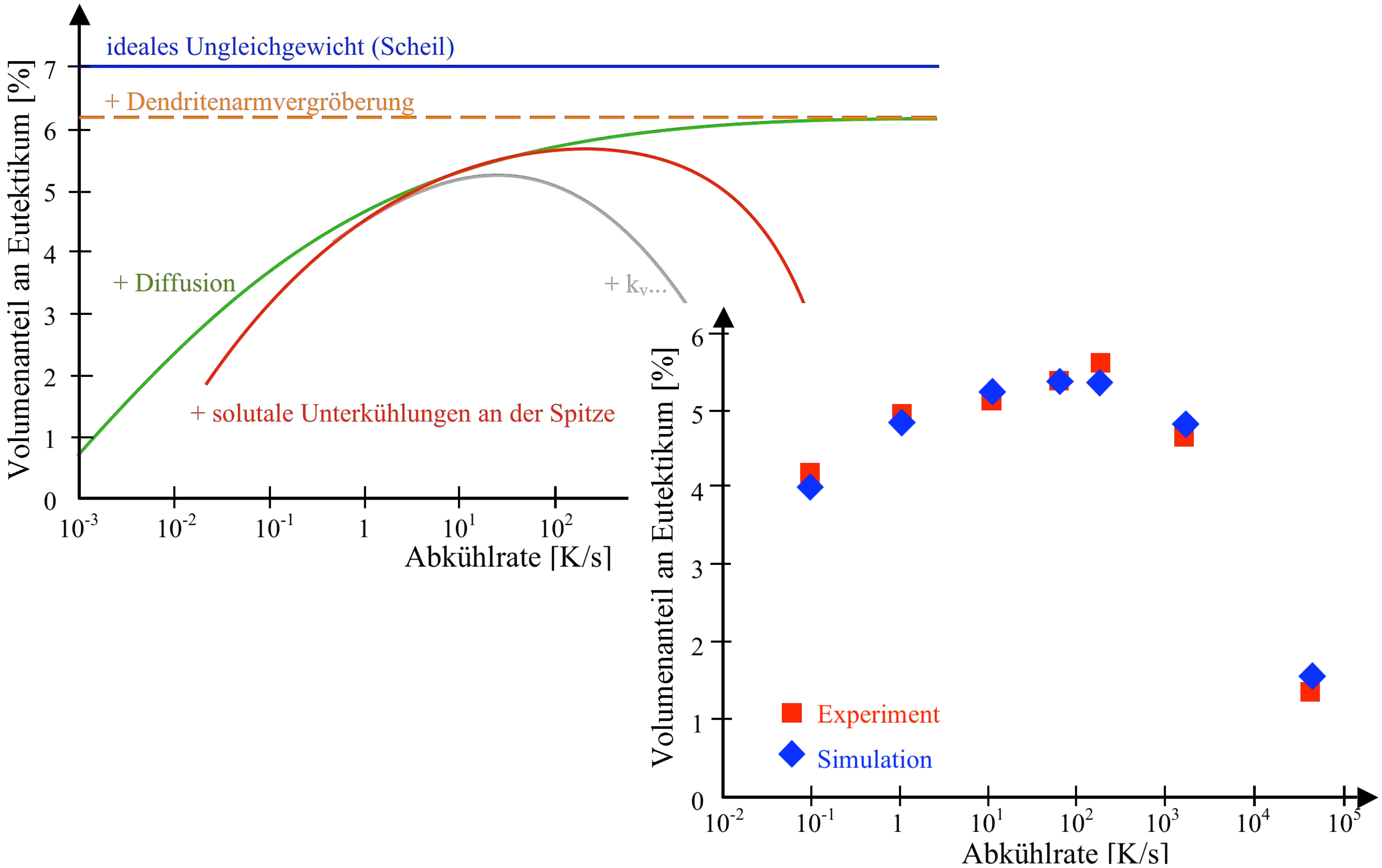
estimated (steepest slope)

calculated $D_{s,Mg} = 0$, $D_{s,Si} = \infty$

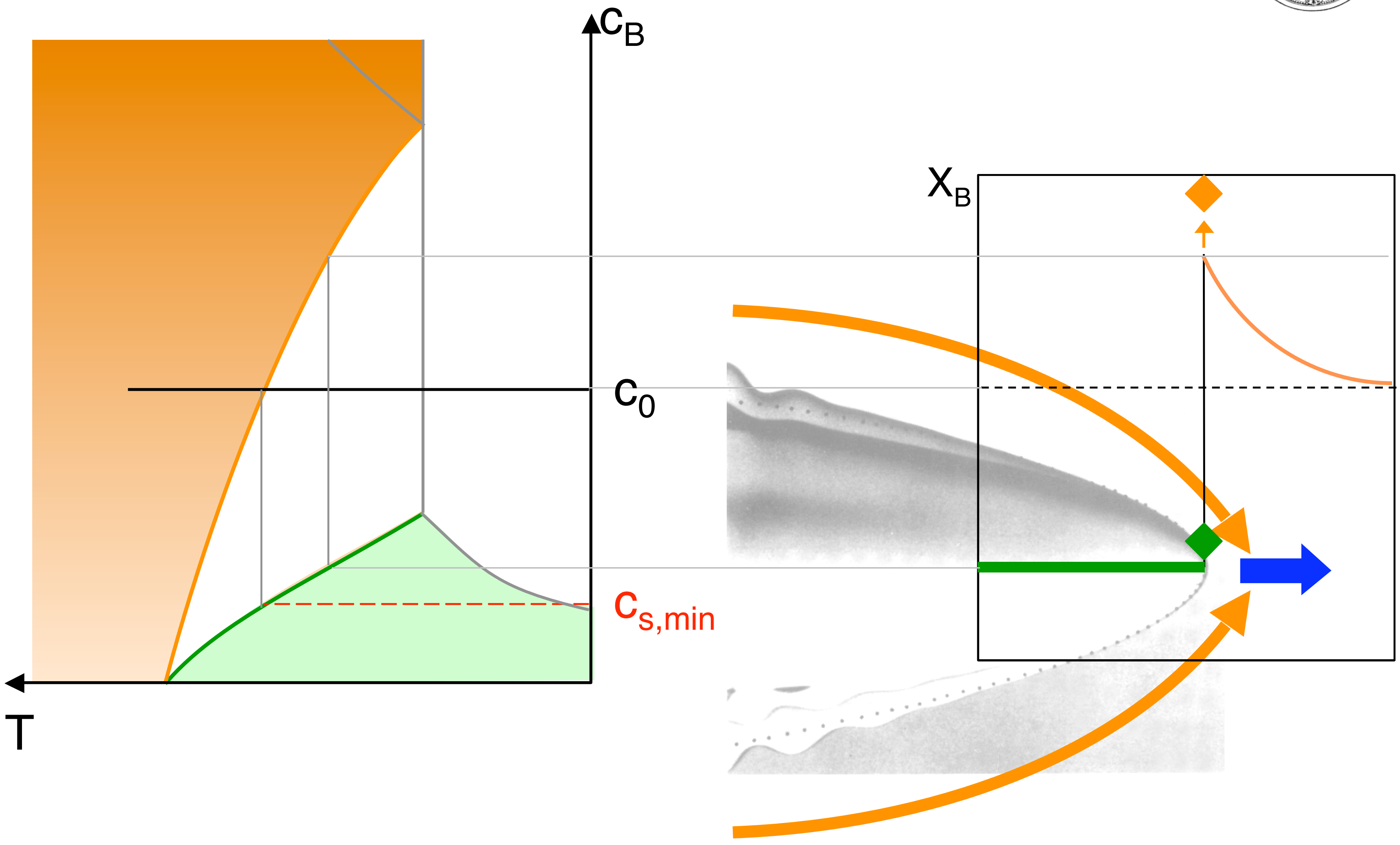
calculated $D_{s,Si} = 0$, $D_{s,Mg} = \infty$



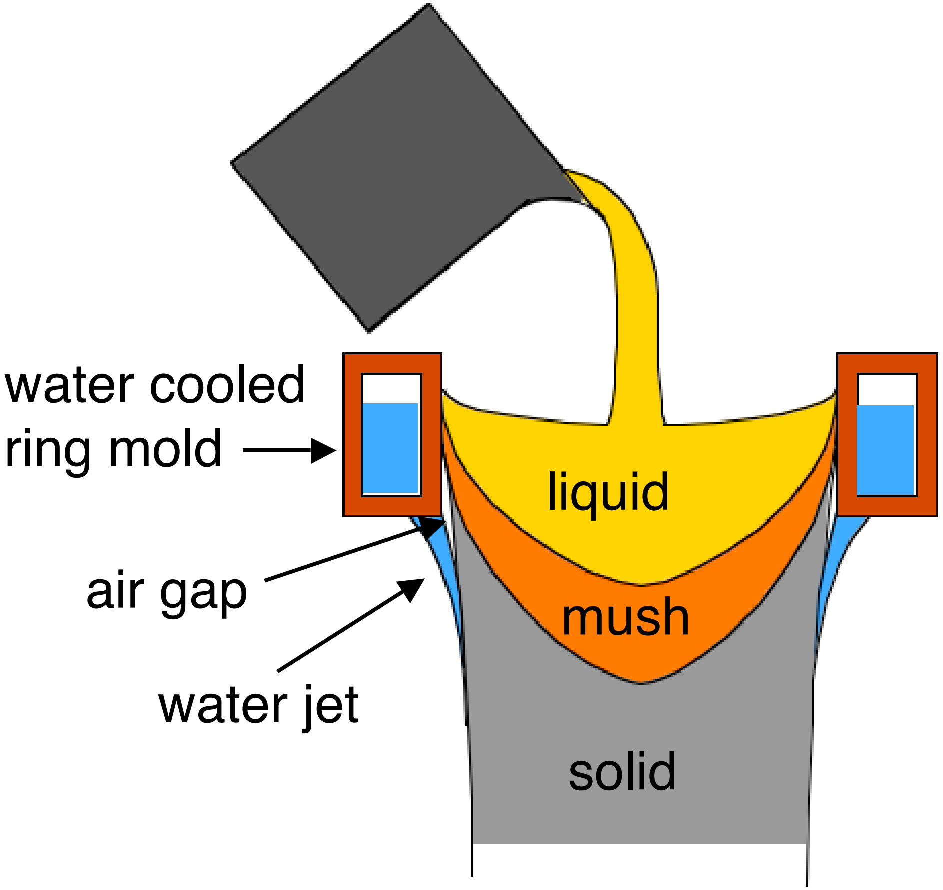
cooling rate and microstructure

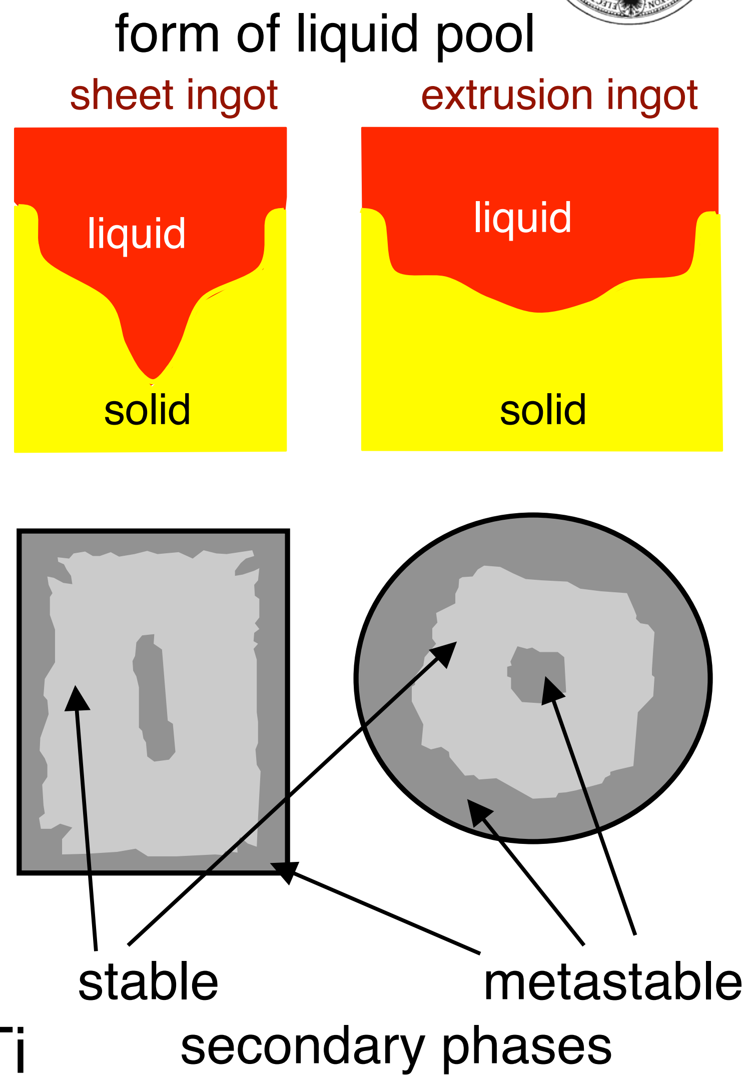


solutal undercoolings



example: DC casting





Materials

Al-0.8Fe-0.8Si

Al-1.3Fe-0.1Si

+ Cu, Mn, Cr, Zn & Ti

Al-Fe-Si phase diagram

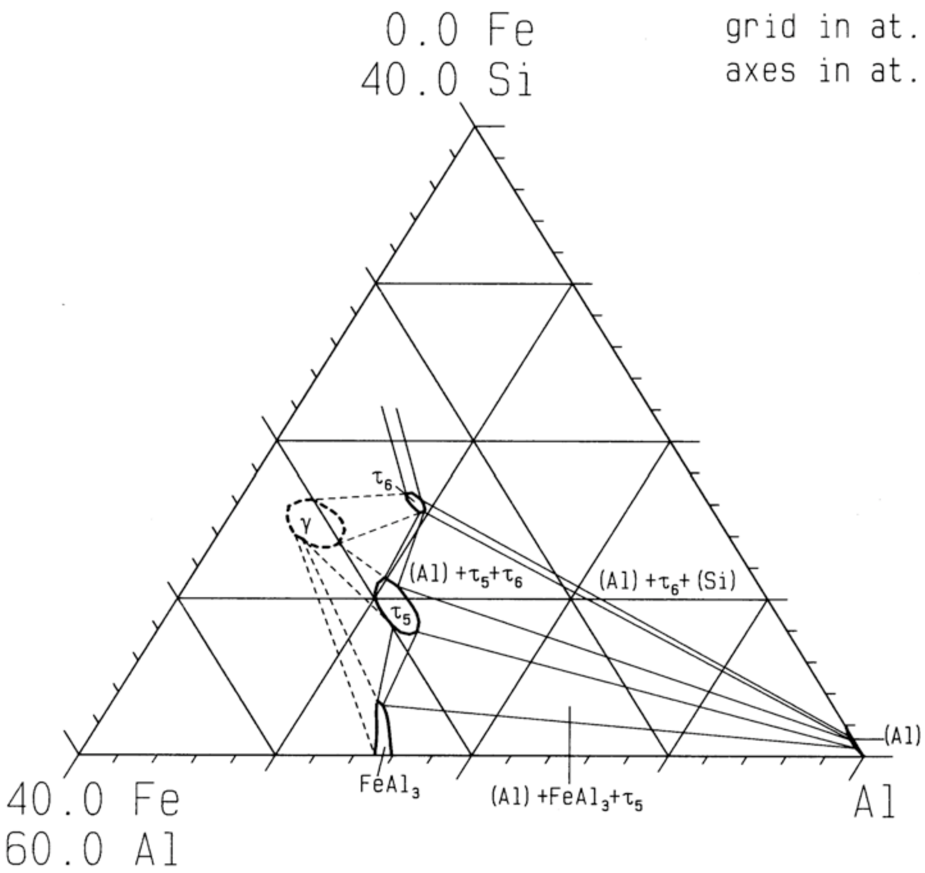


Figure 9: Isothermal section of the Al-corner at 570 °C/600 °C, see text

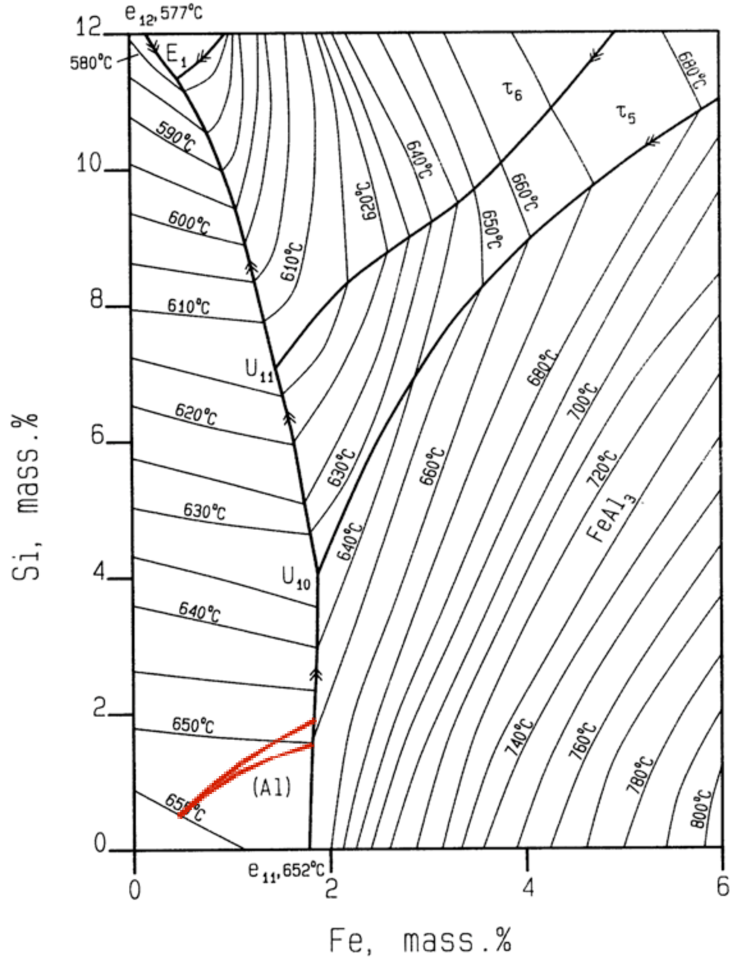
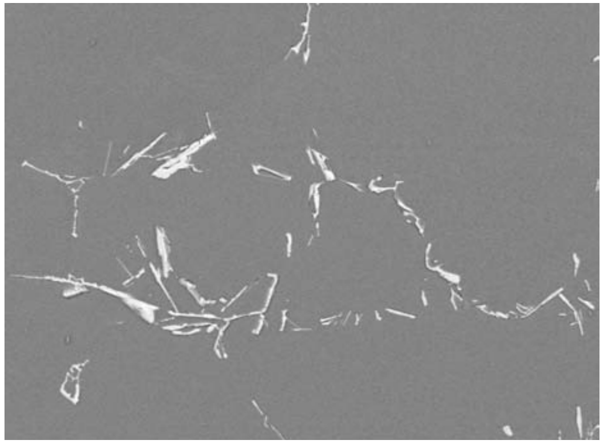
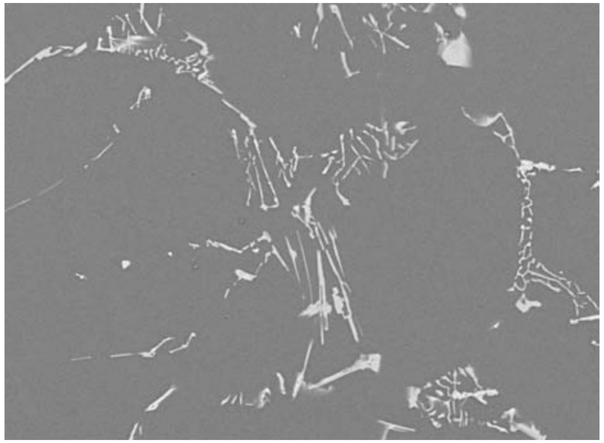


Figure 5: Liquidus surface of the Al-corner of the Al-Fe-Si system

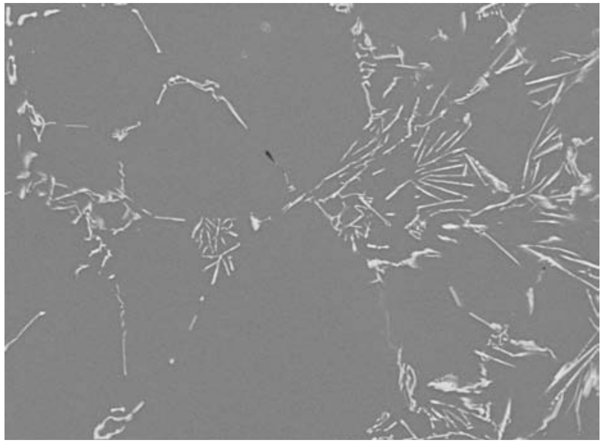
cooling rate and microstructure



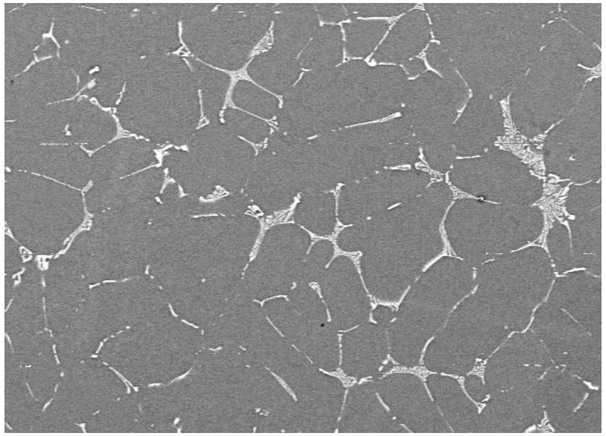
furnace



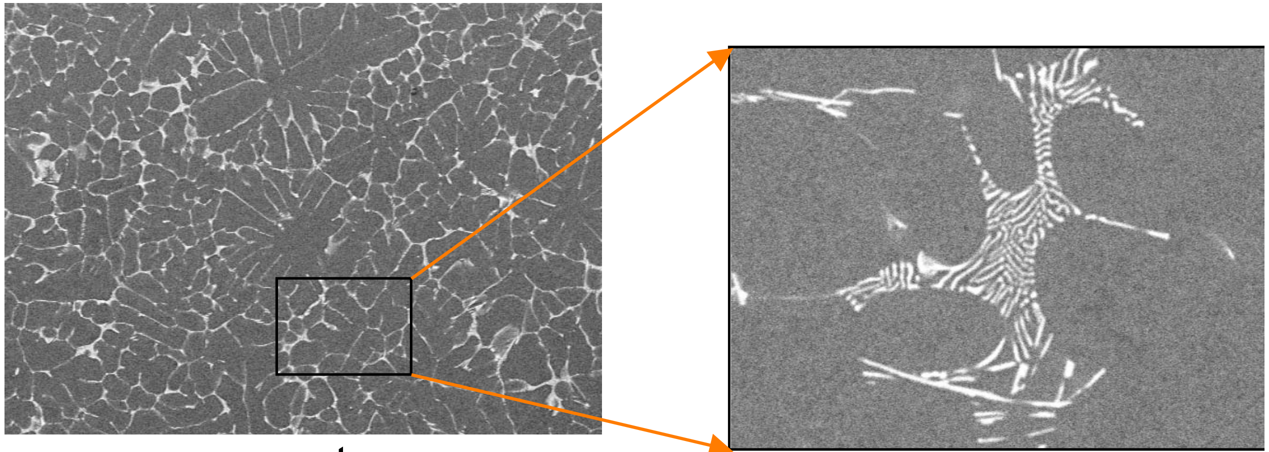
air



forced air

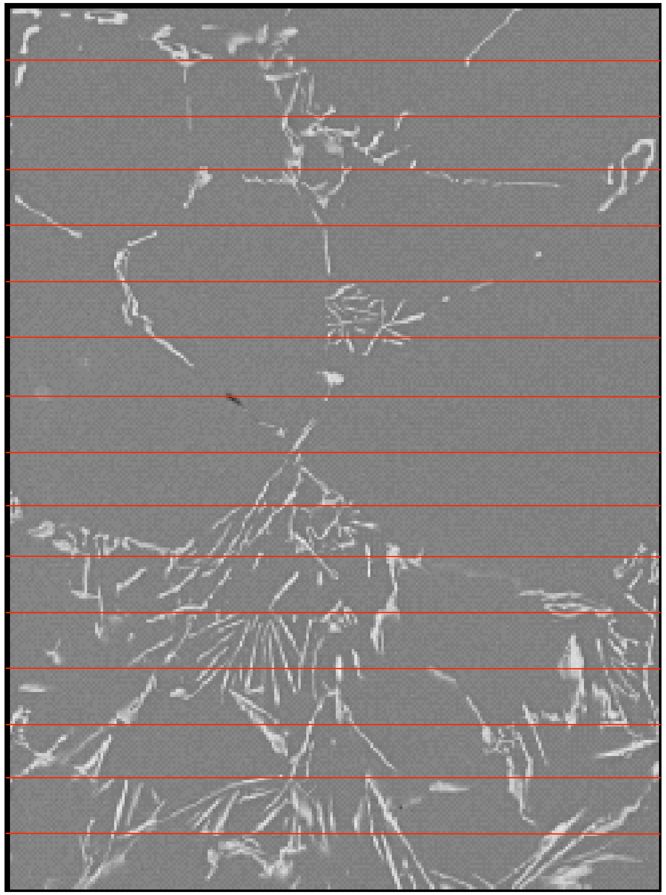


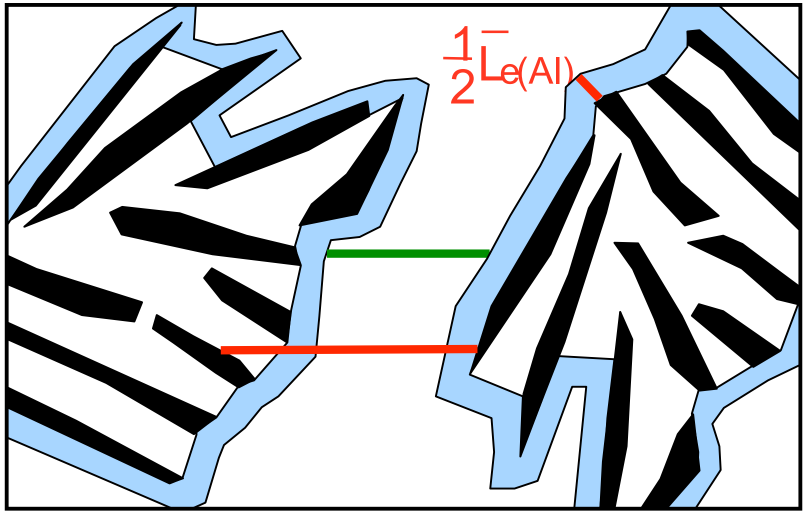
oil

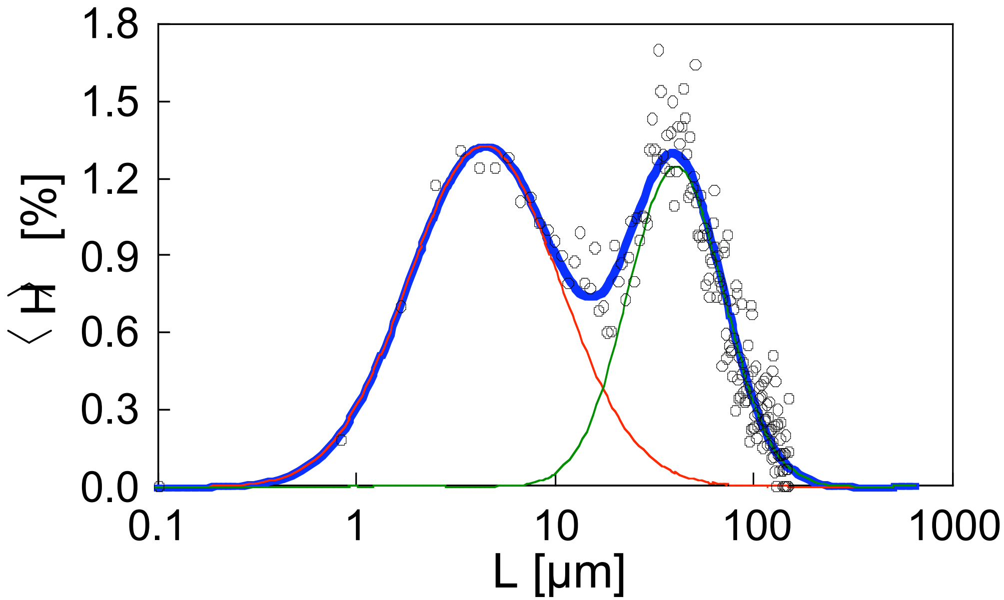


water

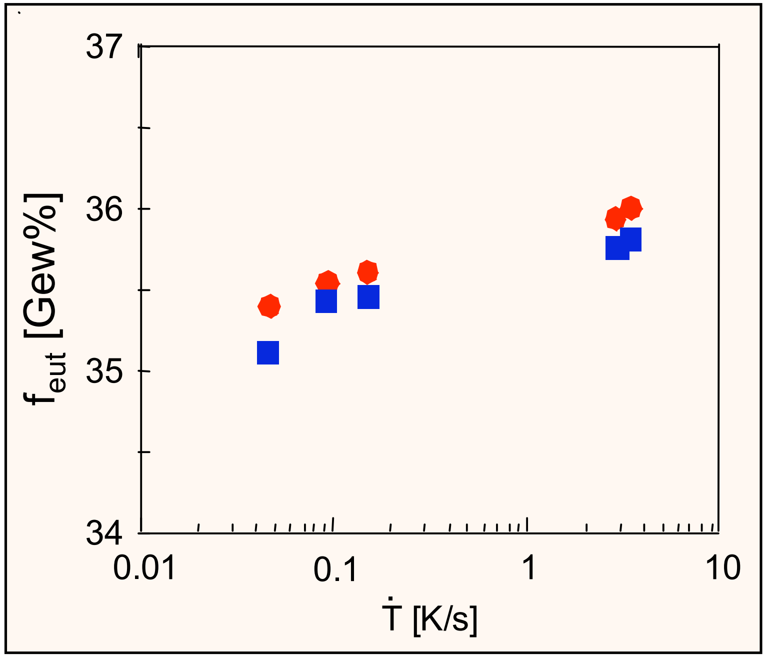
evaluation: image analysis

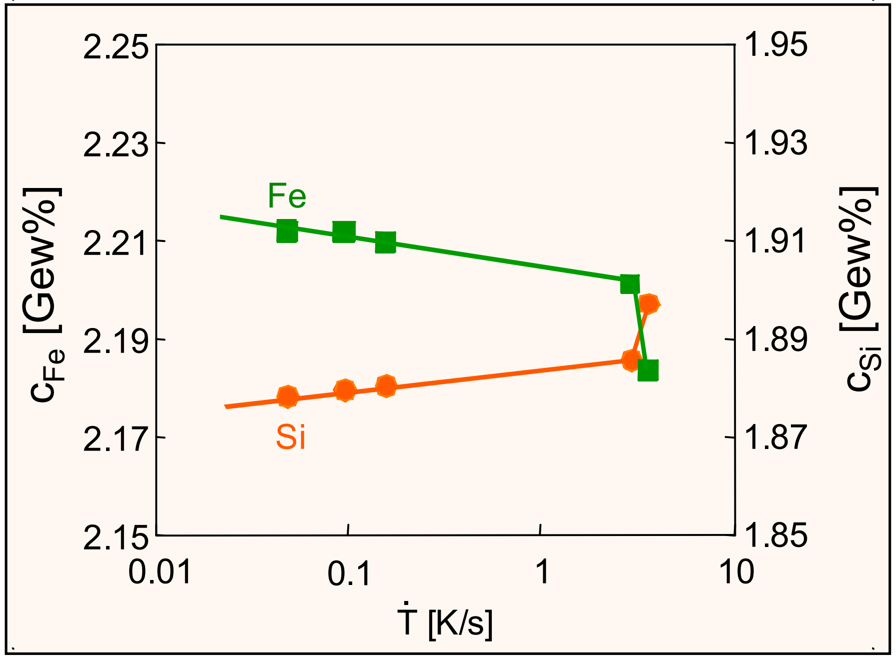






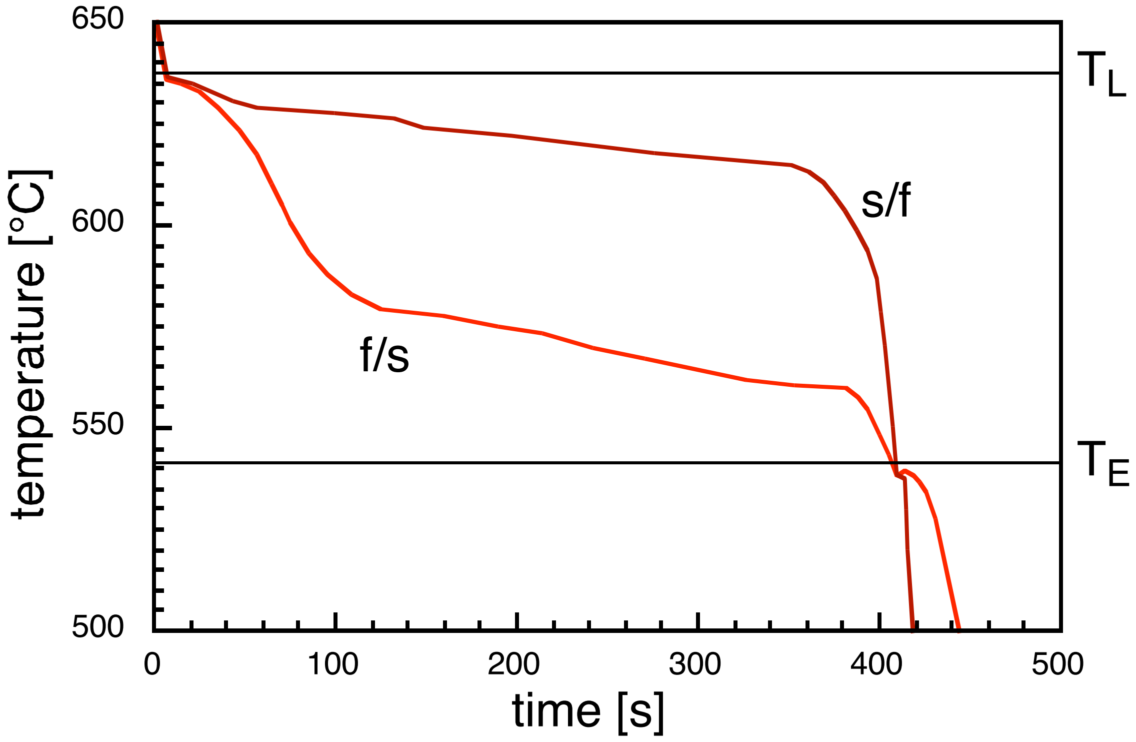
experiment and simulation

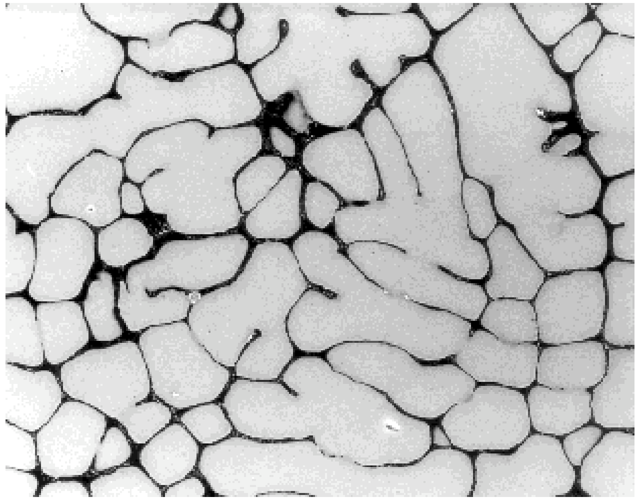


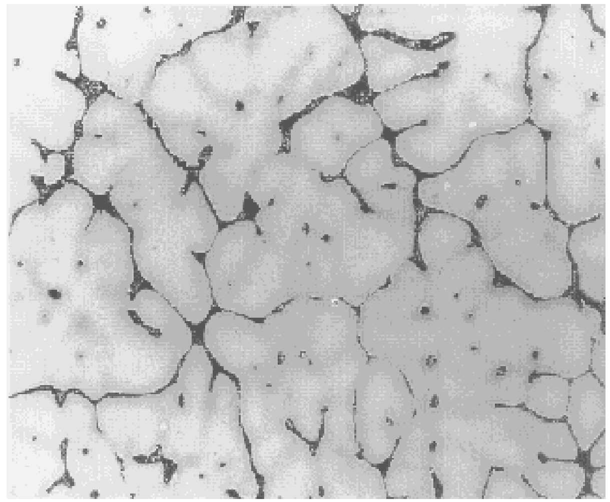


consequences ?

- reduce segregation, e.g. by cooling schedule
- optimize annealing time







eutectic fractions

	measured	calculated
s/f	12.0	12.2
lin	10.9	10.7
f/s	9.6	9.6

conclusions

reliable phase diagrams are a prerequisite for solidification simulation
kinetic calculations are not meaningful if phase diagram is only estimated

visualization (2D-simulation) is a tool for better understanding
but: beautiful pictures do not imply accuracy or scientific profoundness

accurate predictions of phase fractions are possible
measurements are as tedious as modelling
both lever rule and *analytical* Scheil equations are not sufficient
⇒ apply Scheil *conditions* ($D_s = 0$, $D_\ell = \infty$) and CALPHAD

technically important features can be determined
qualitative predictions most important (solidifying phases, solidification path)
quantitative predictions for design of further processing steps