Scheil or Lever Rule?

modelling of kinetics during solidification

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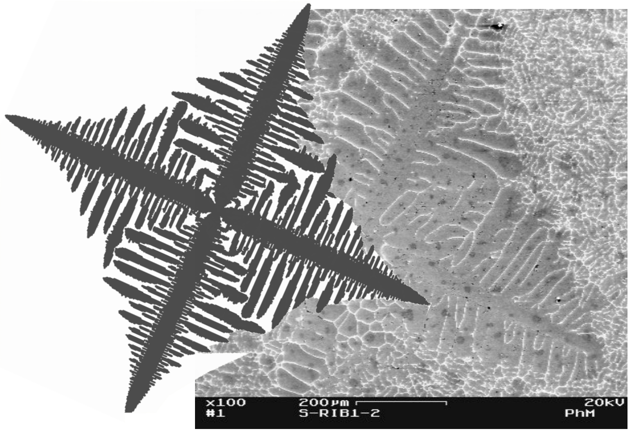
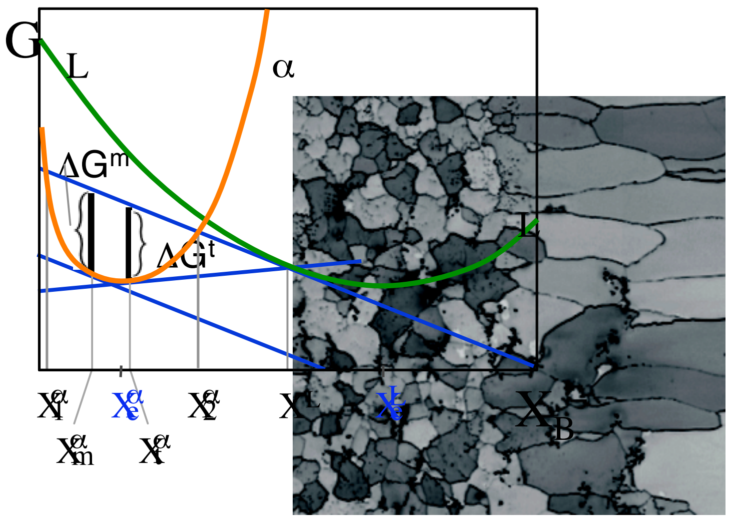
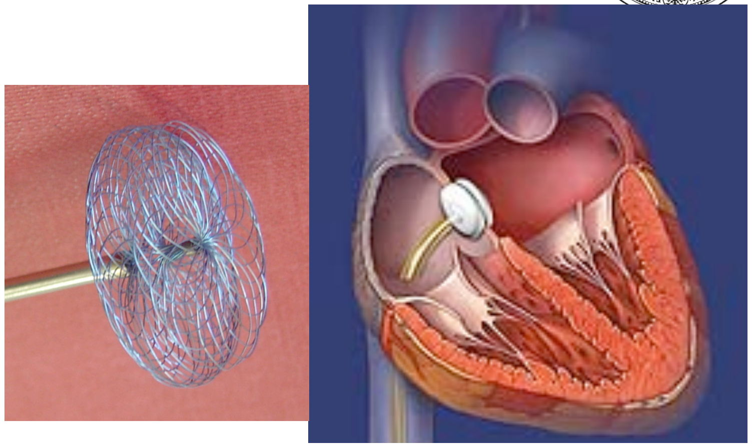
research fields

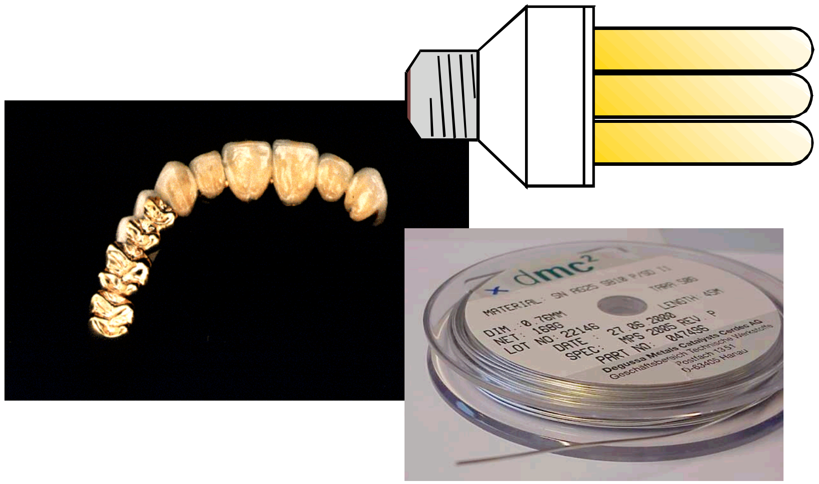


structure formation
(non-equilibrium) thermodynamics





implant alloys



alloy development

outline

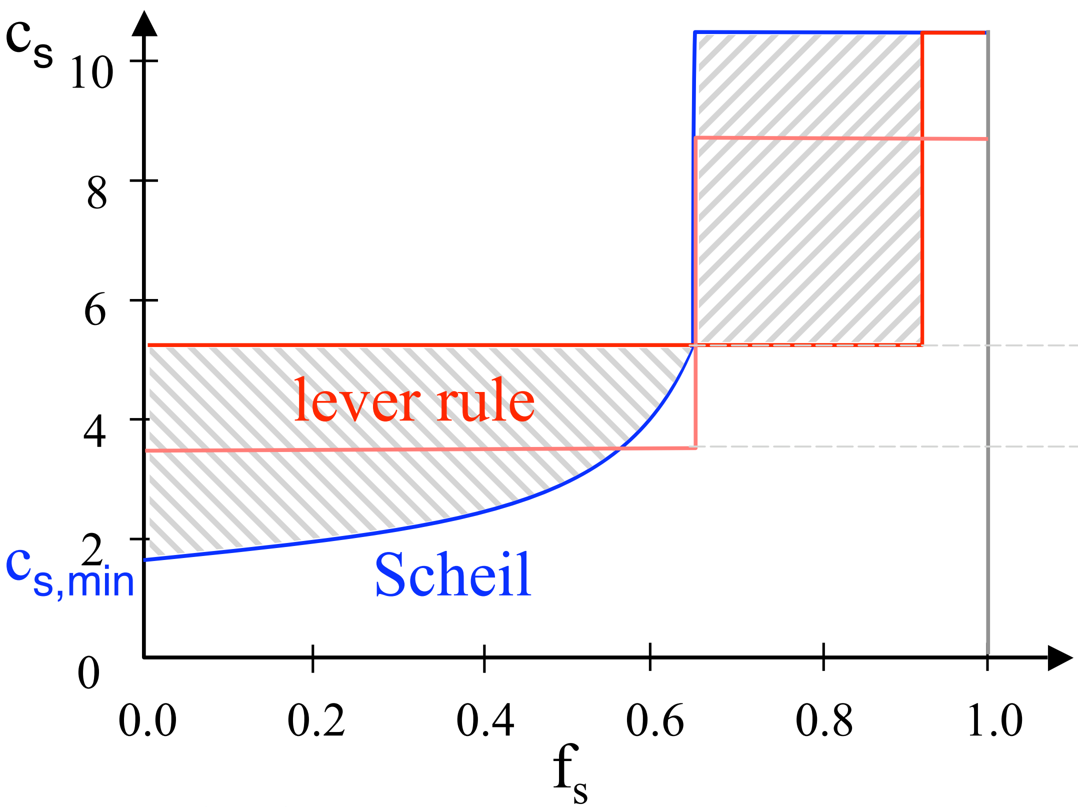
Reminder: Scheil and lever rule

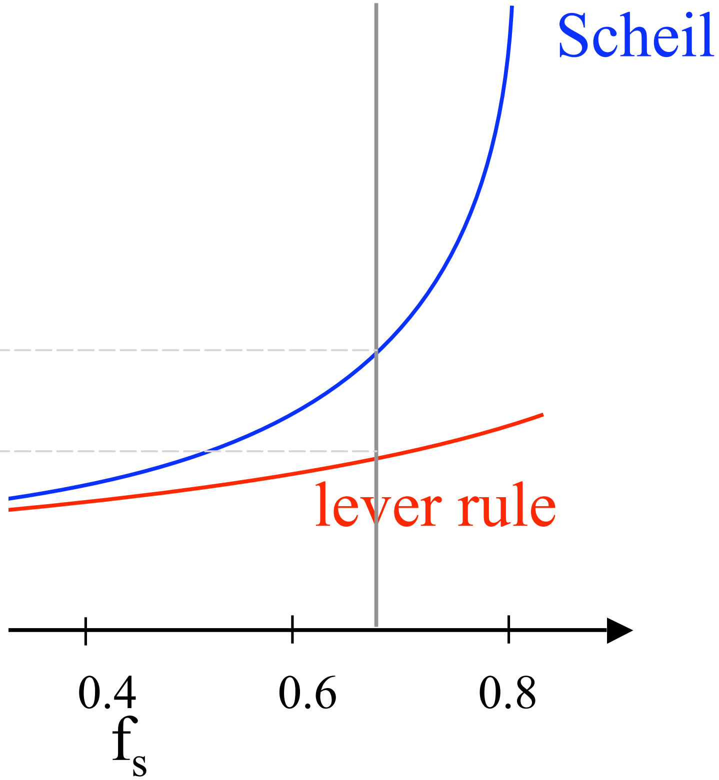
Microsegregation model SolKin
- coarsening
- growth undercoolings

Limits of Scheil and lever rule, binary and multicomponent alloys
- solidification path
- concentration distribution

Example: Al-Fe-Si

Lever rule and Scheil conditions





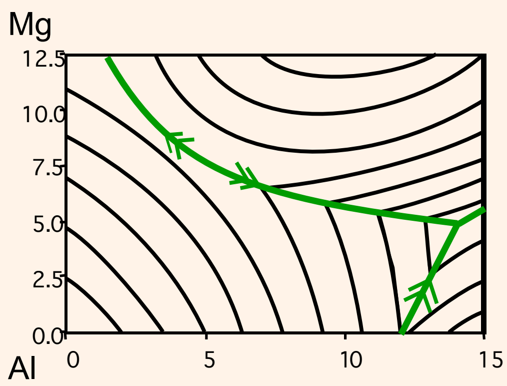
Scheil:

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

Scheil: $c^*(t)$ and $c(x)$

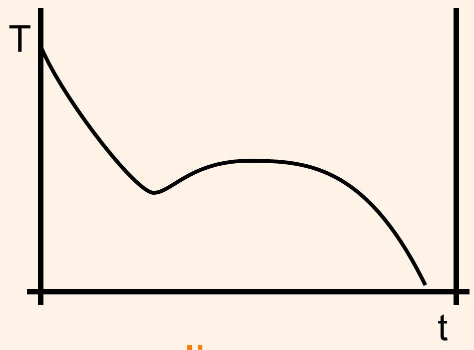
lever rule: $c^*(t)$

microsegregation model SolKin

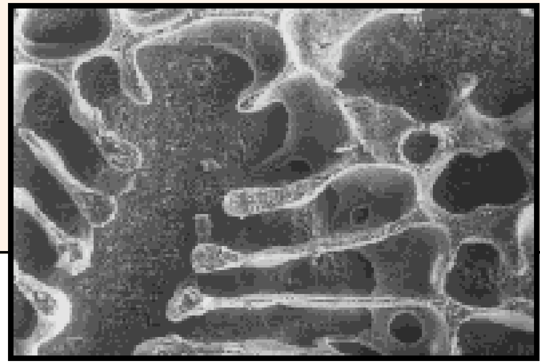


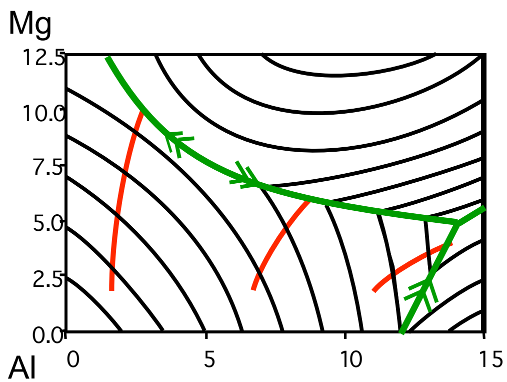
phase diagram
(tie lines)

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

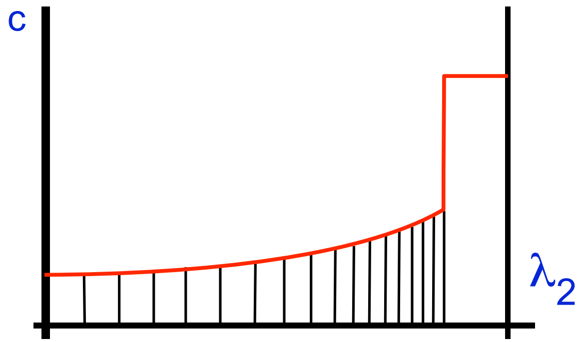


cooling curve

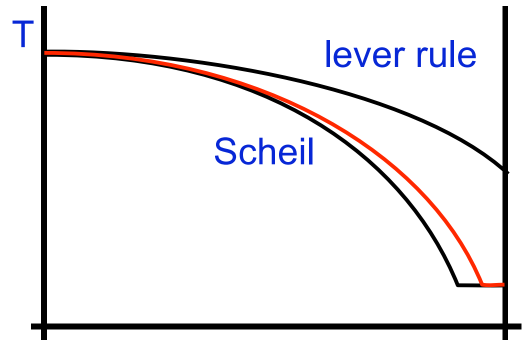




solidification path

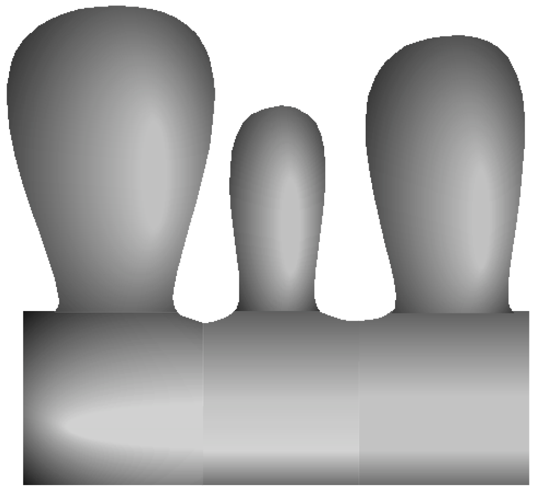


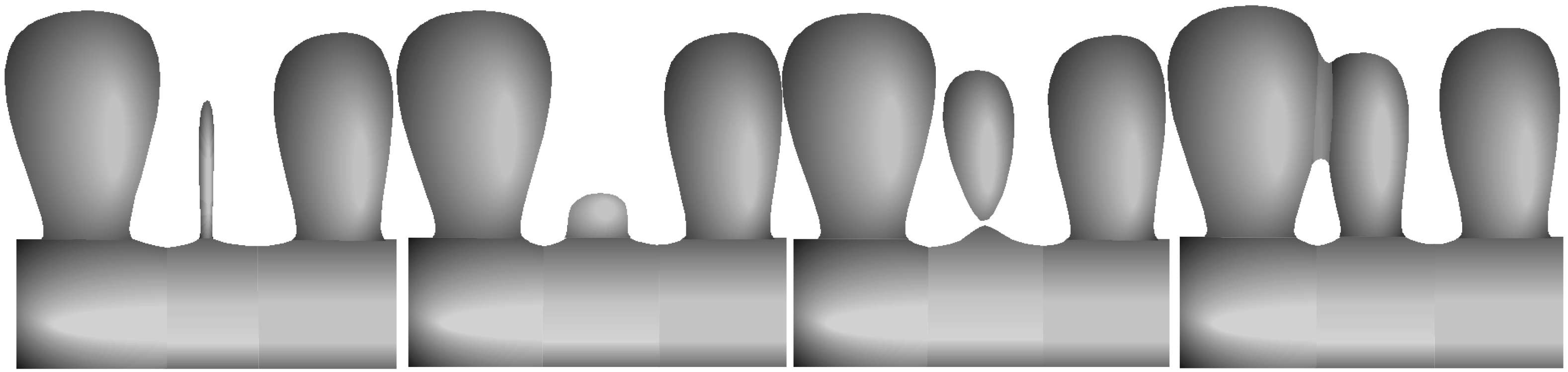
concentration profile
phase fractions



solid fraction
solidification temperature

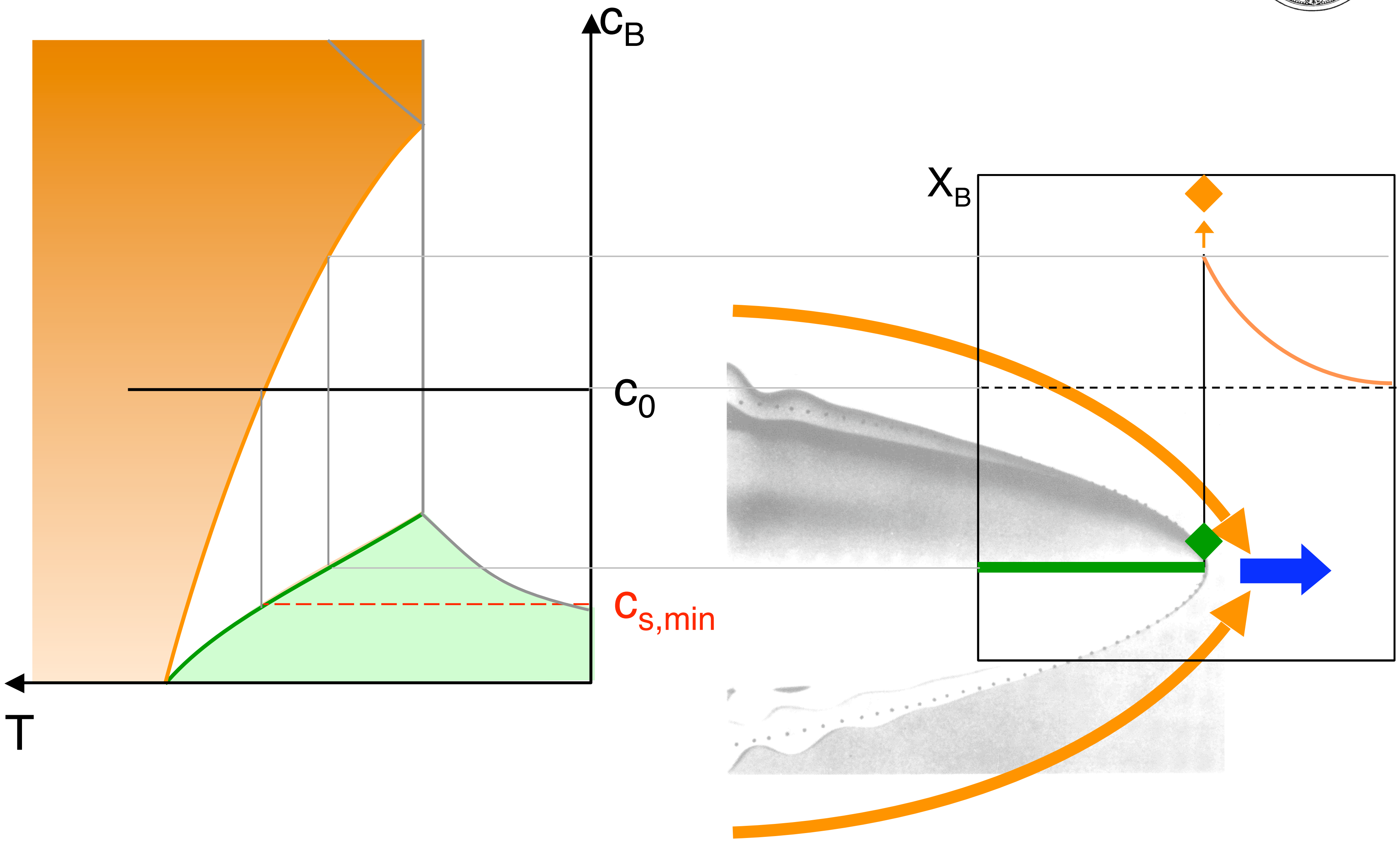
coarsening



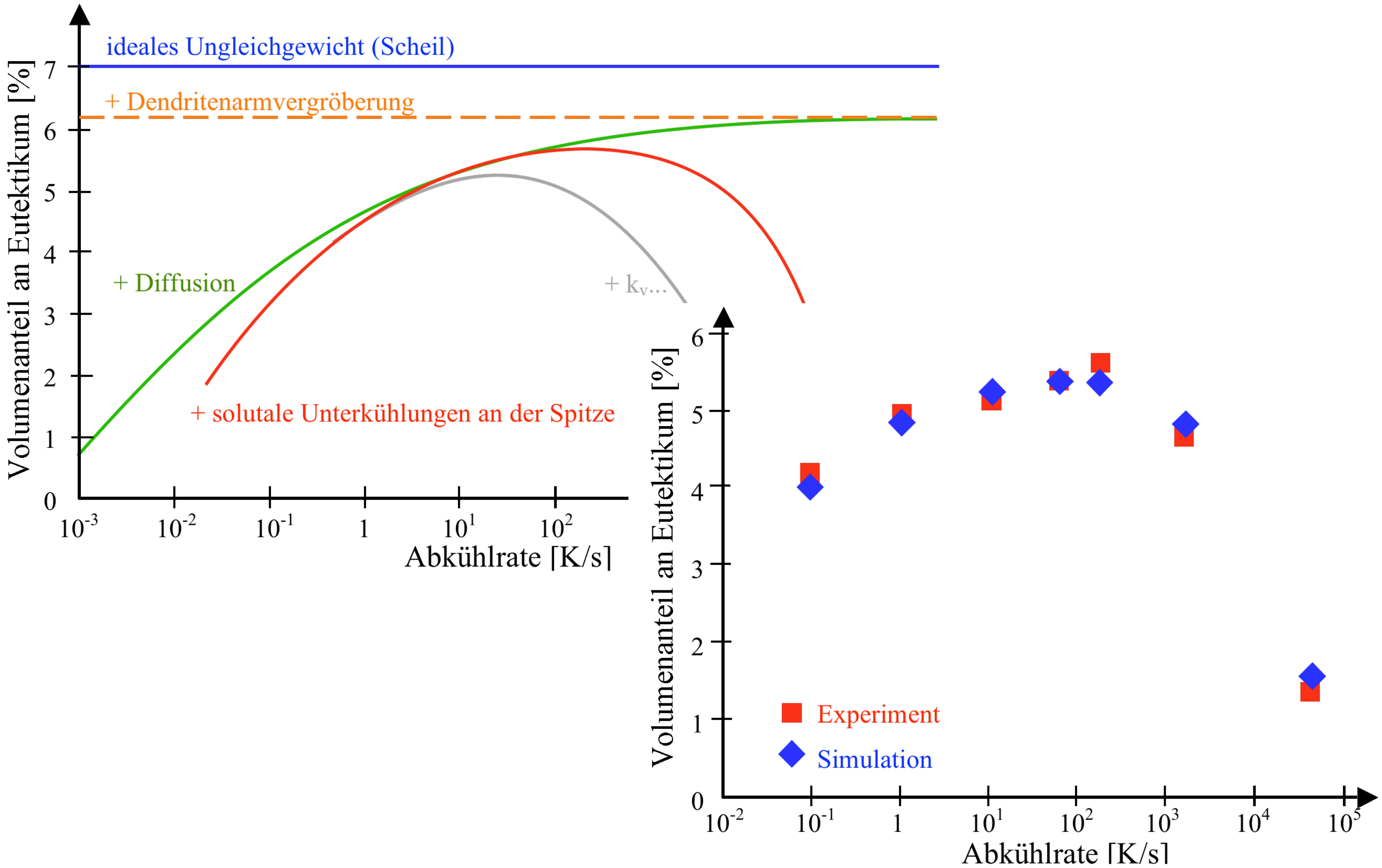


radial melting   axial melting   melting at root   coalescence

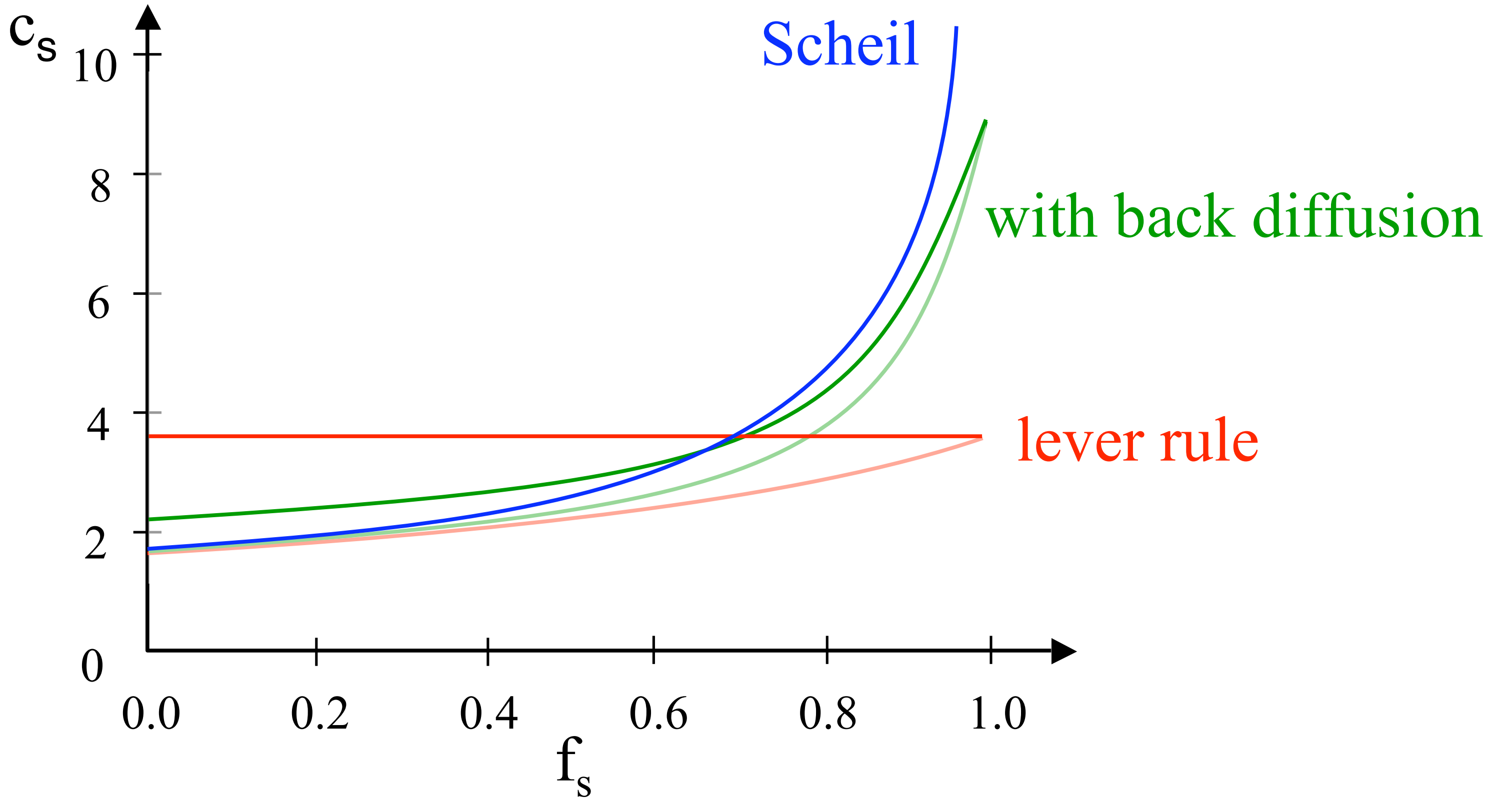
growth undercoolings



cooling rate and microstructure



real profiles between idealized ones?



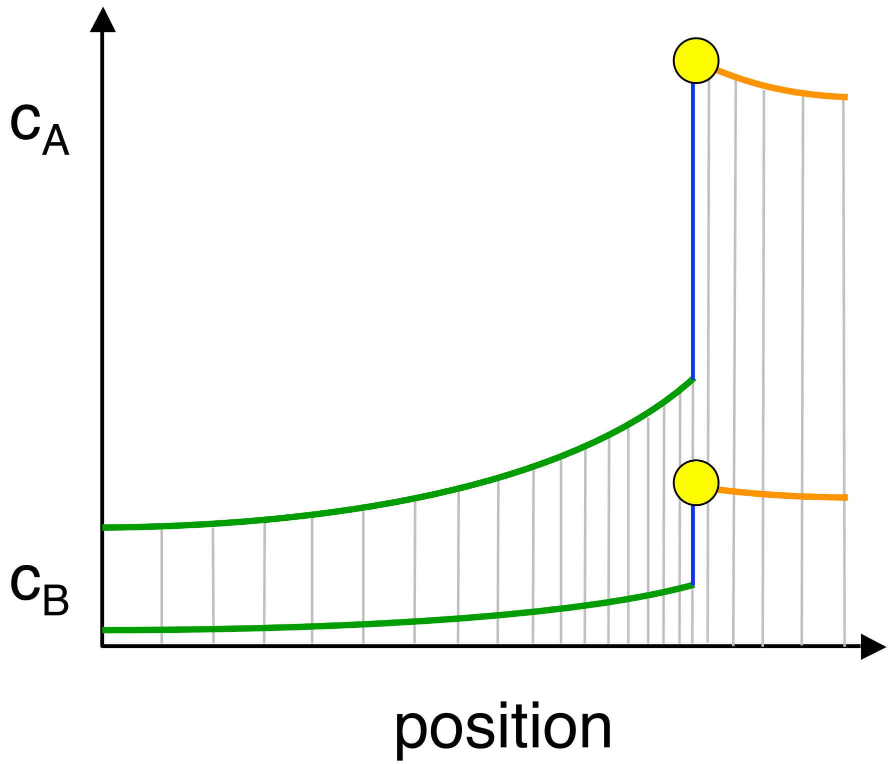
binary alloys:

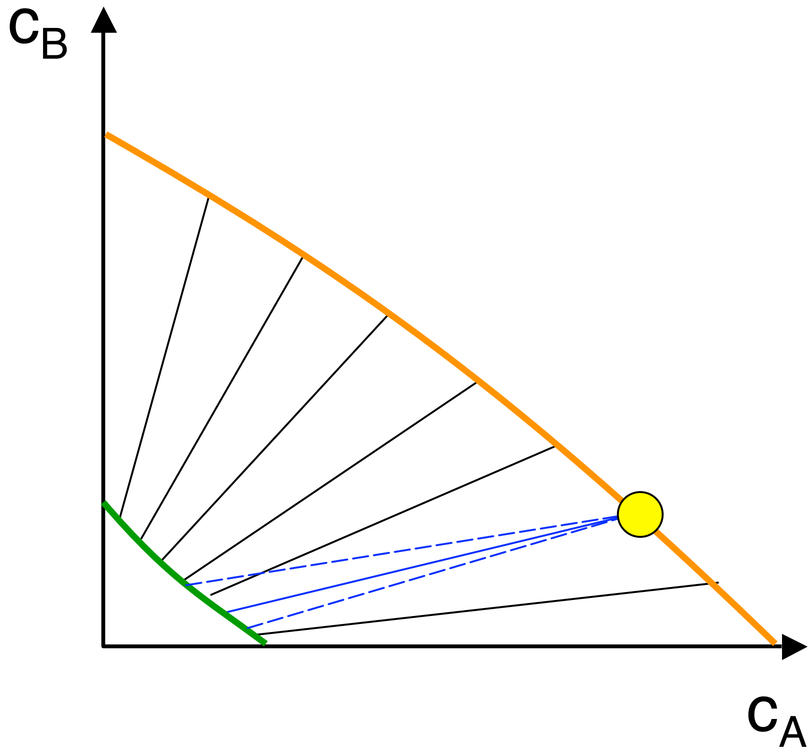
- realistic **interface concentrations** between Scheil and lever rule
- realistic concentration profiles not necessarily between Scheil and lever rule

coupling with phase diagram

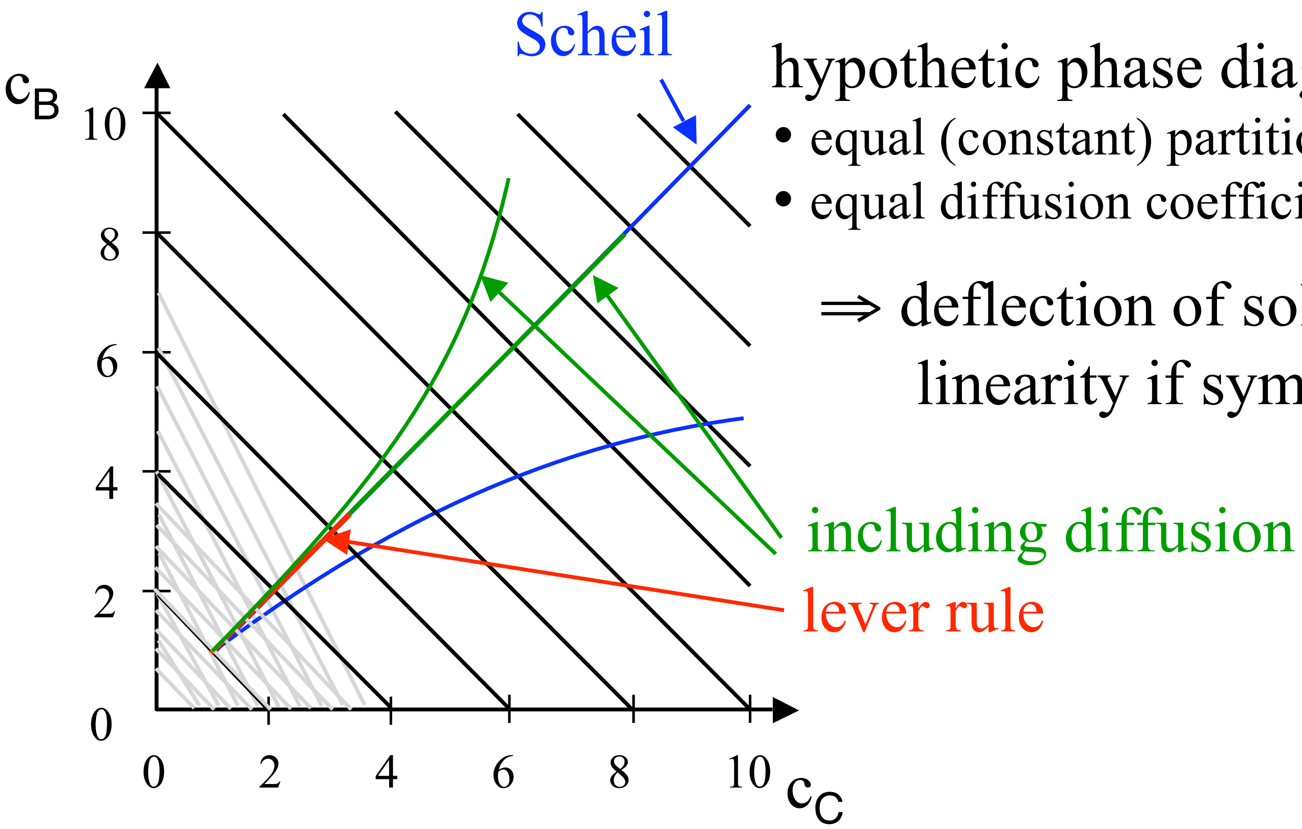
- binary alloys: interpolate phase boundary lines
- ternary or higher alloys: more degrees of freedom
- analytical solutions (‘multibinary‘) fail
- Scheil equation ⇒ Scheil **conditions**

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





real solidification paths between idealized ones?



hypothetic phase diagram:

- equal (constant) partitioning of elements B and C
- equal diffusion coefficients of B and C

⇒ deflection of solidification path from linearity if symmetry is broken

ternary or multicomponent alloys:

- solidification paths my lie on top of each other
- **difference** of kinetic coefficients sets limits of solidification path

solidification paths:

estimated (steepest slope)

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

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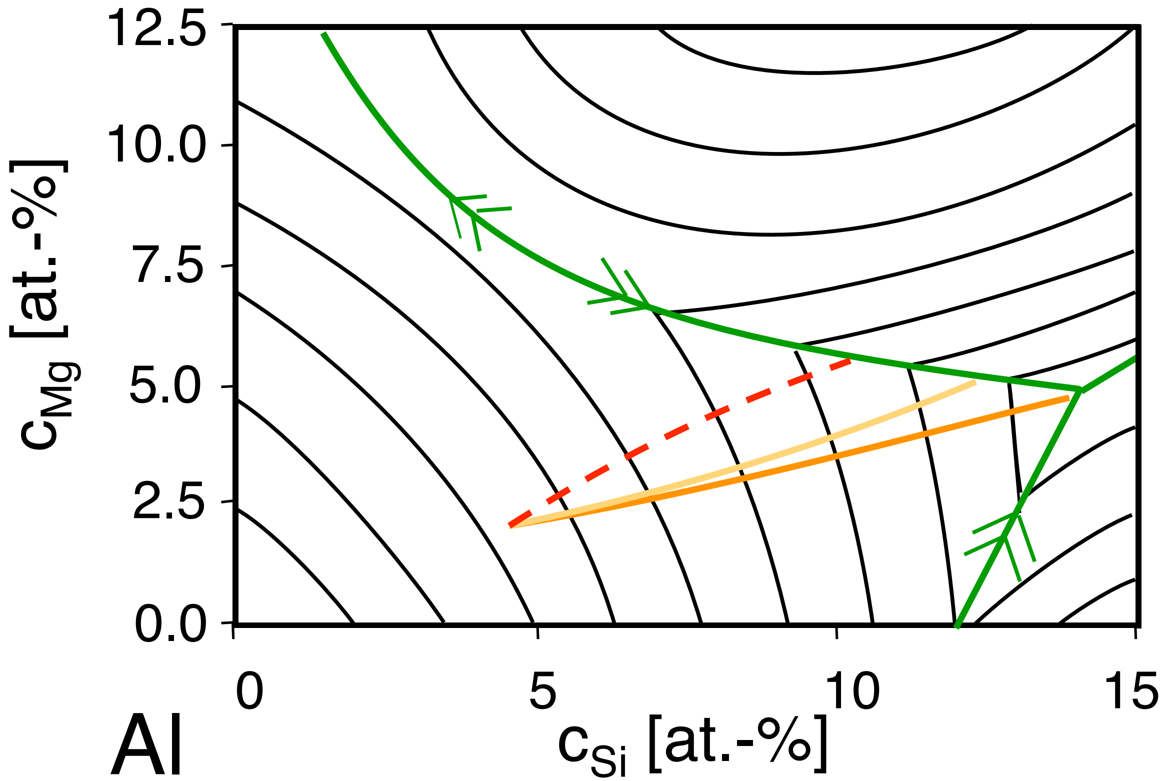
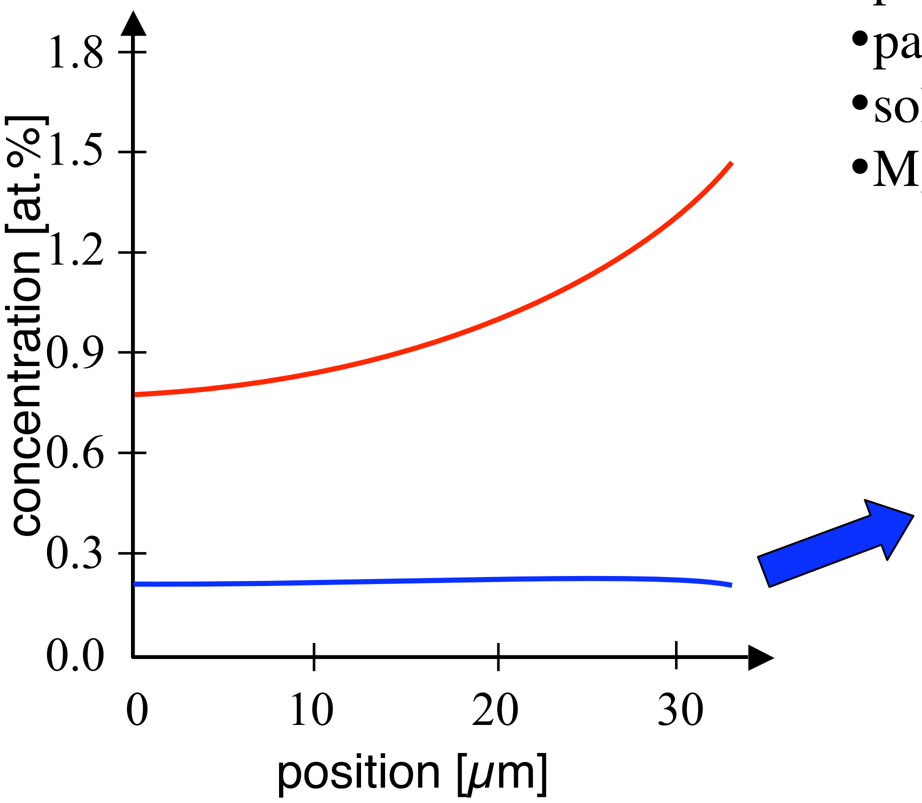


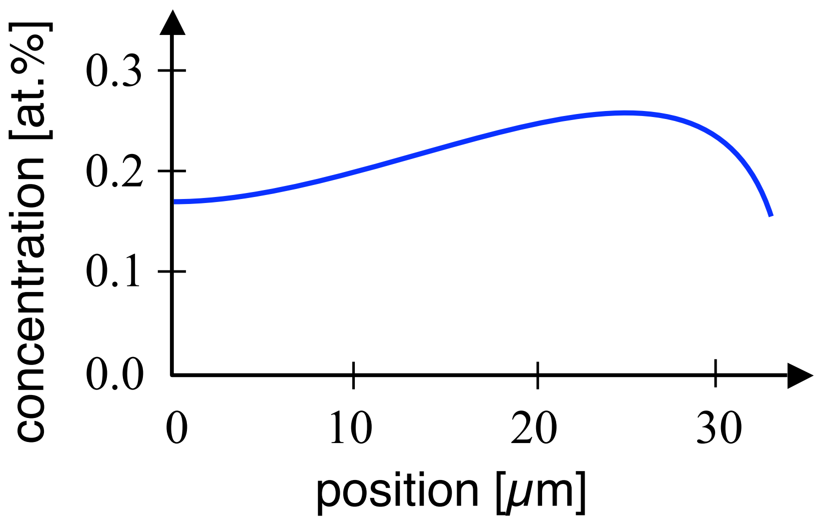
real concentration profiles between idealized ones?

Al-Mg-Si:



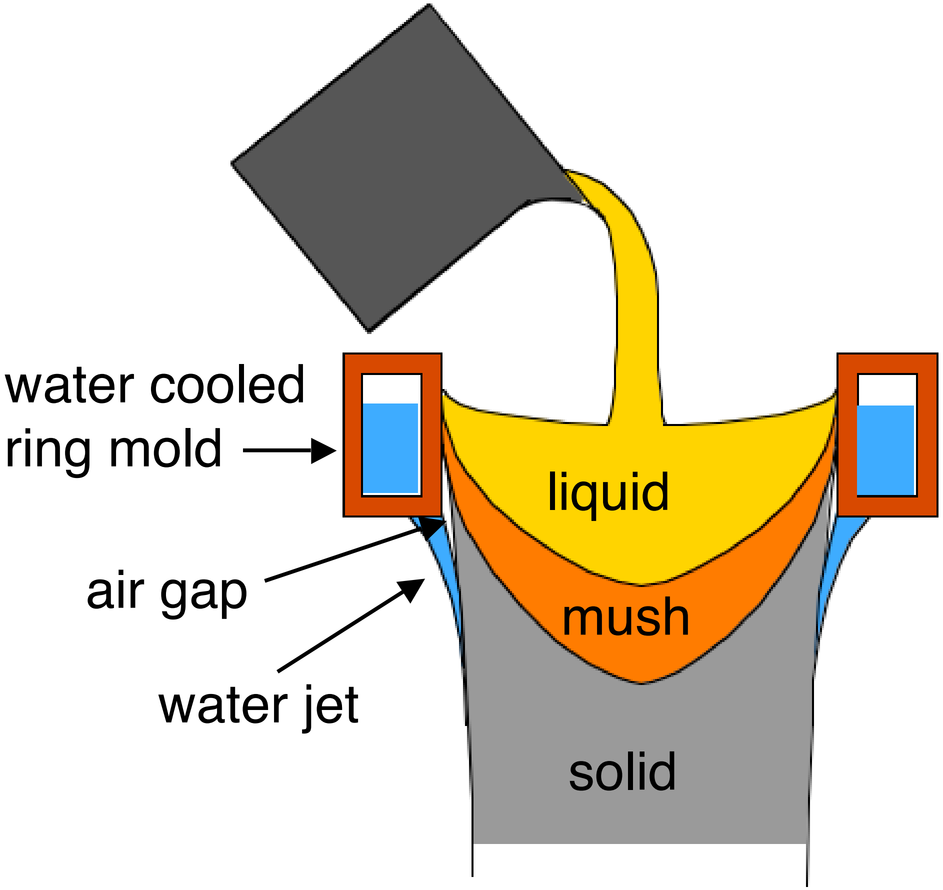
realistic concentration distribution:

- partitioning Si similar as in Al-Si
- partitioning of Mg dependent on Si
- solidification path dependent on kinetics
- Mg solidifies ± segregation free

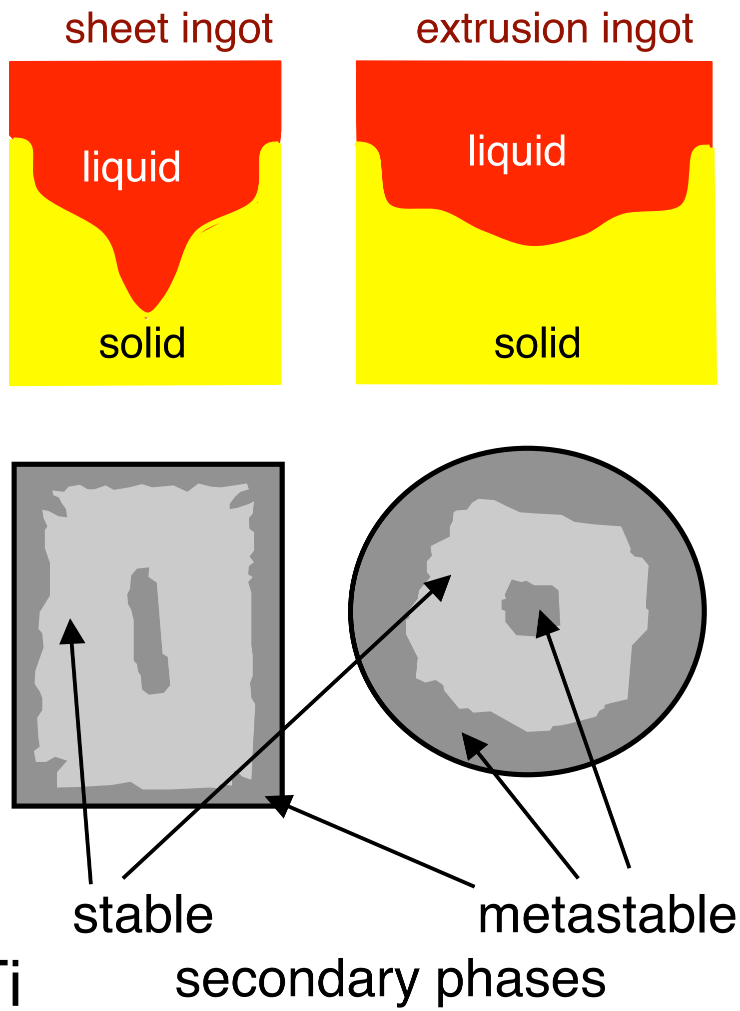


- realistic interface concentrations not neccessarily between Scheil and lever rule
- realistic concentration profiles not necessarily between Scheil and lever rule

example: DC casting



form of liquid pool



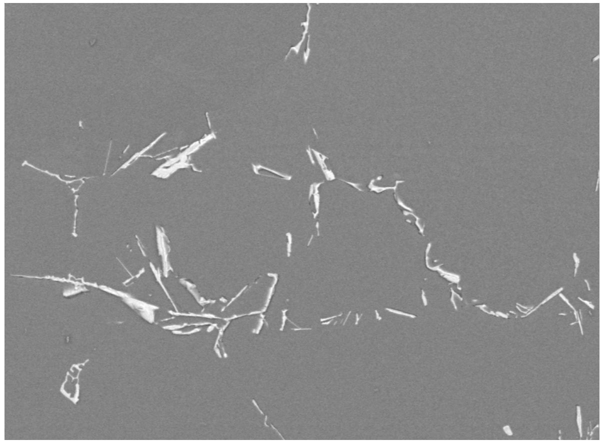
Materials

Al-0.8Fe-0.8Si

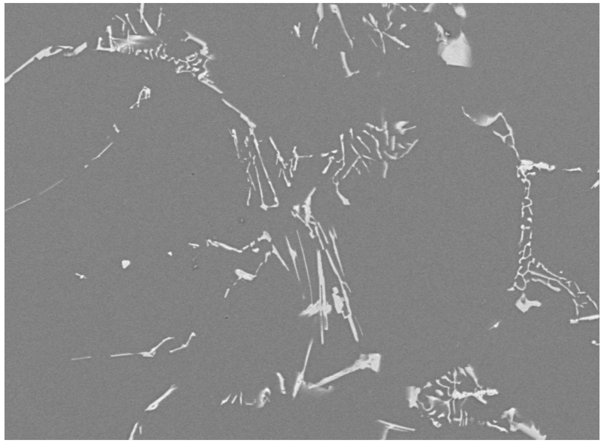
Al-1.3Fe-0.1Si

+ Cu, Mn, Cr, Zn & Ti

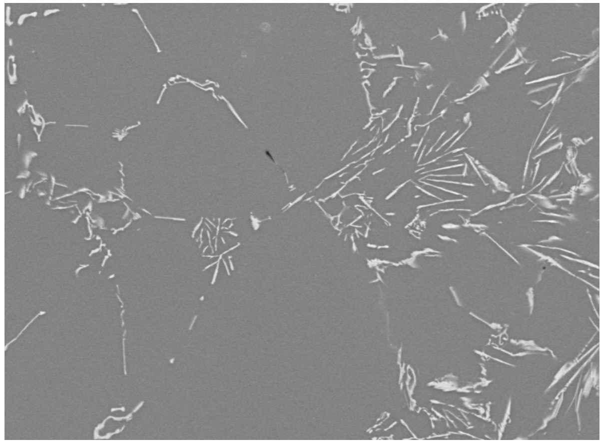
cooling rate and microstructure



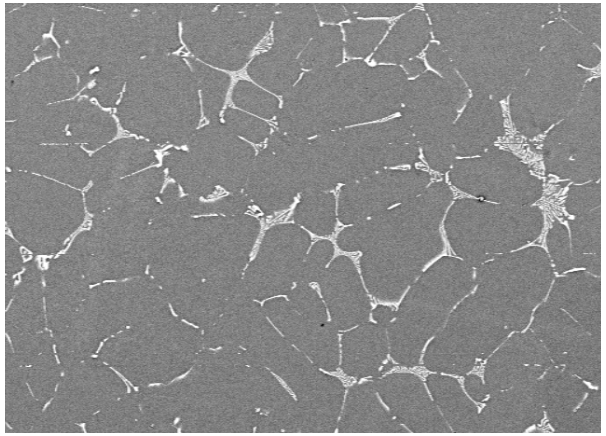
furnace



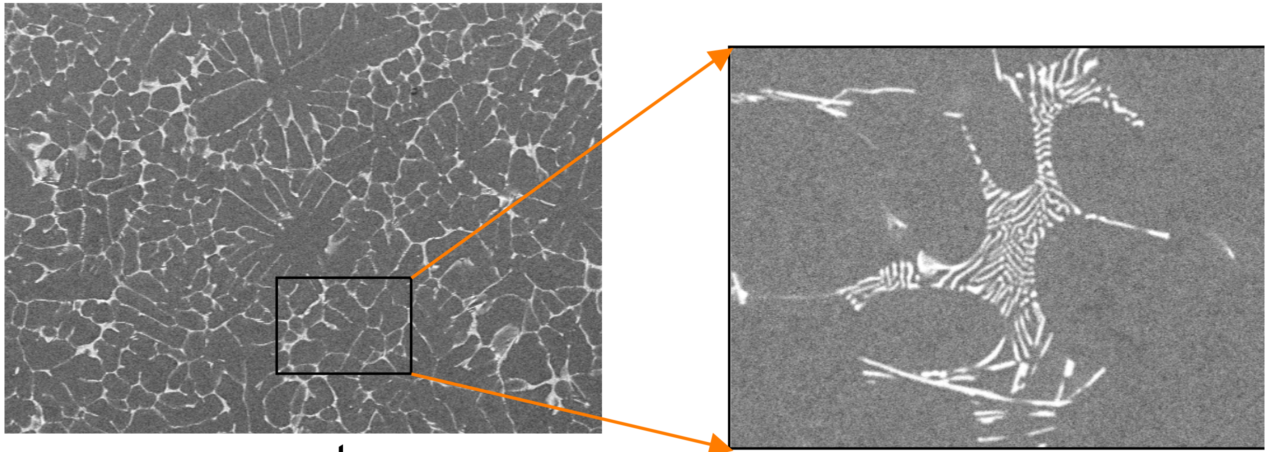
air



forced air

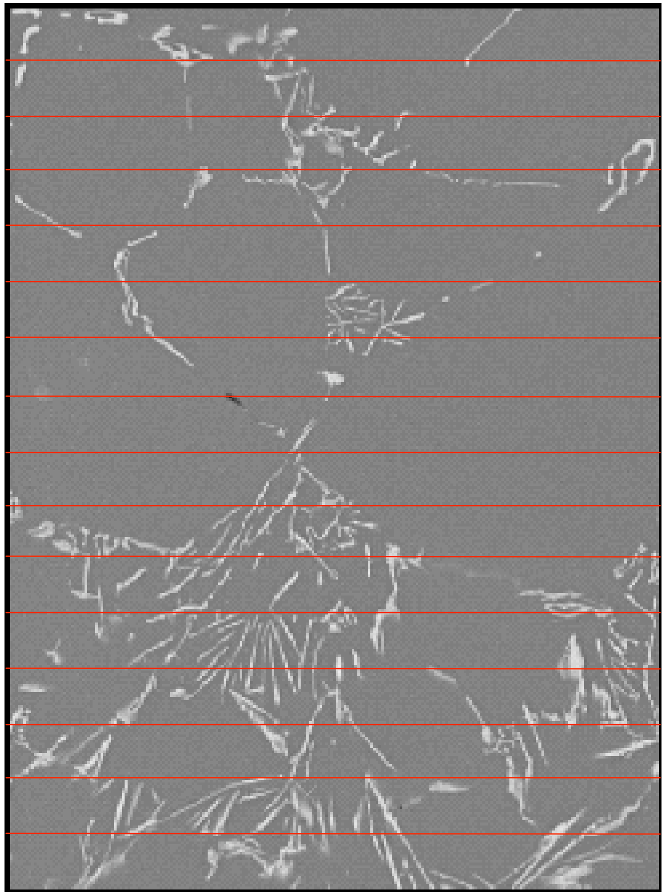


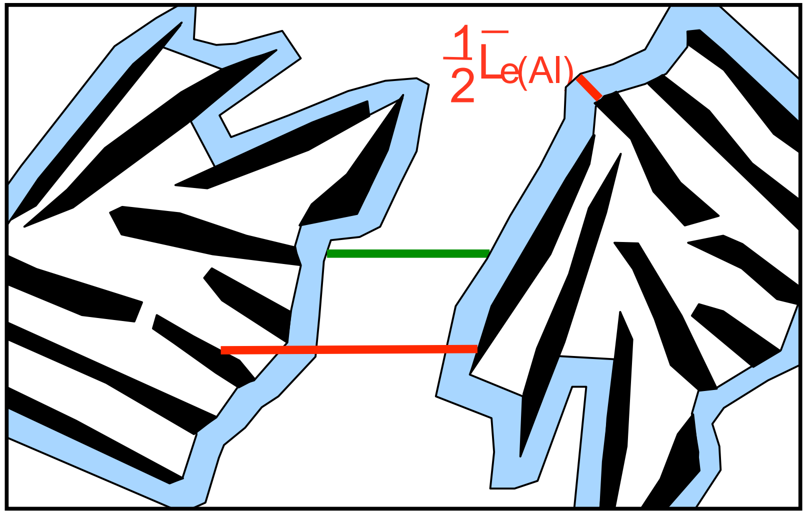
oil

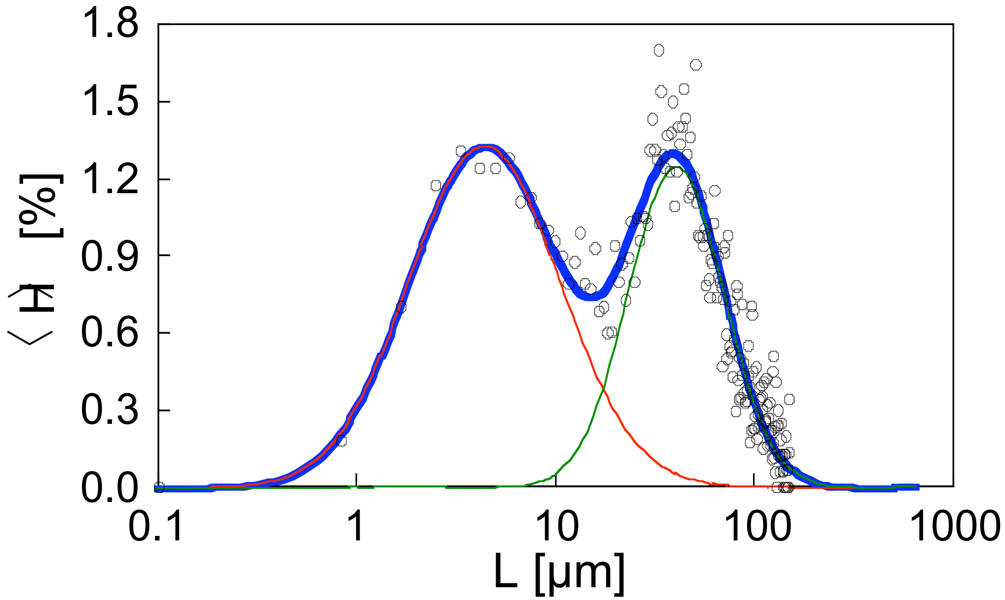


water

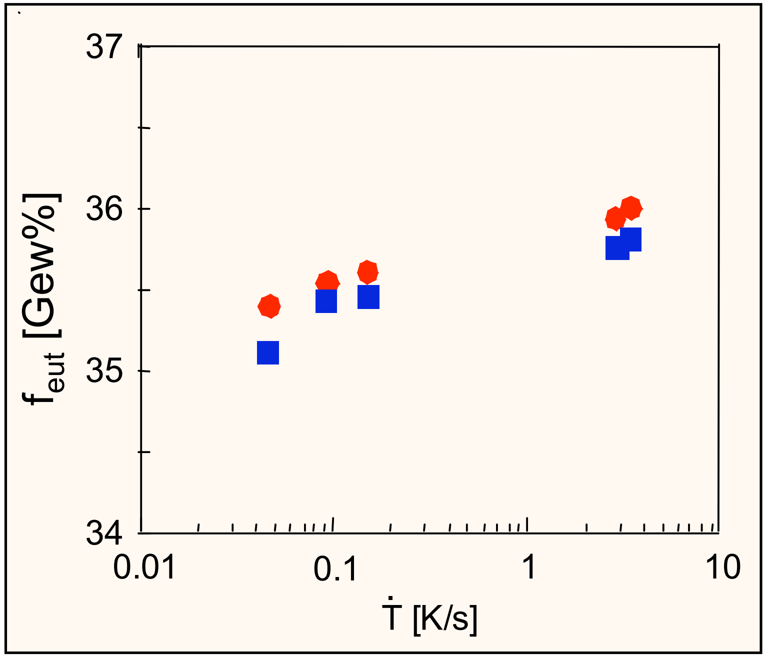
evaluation: image analysis

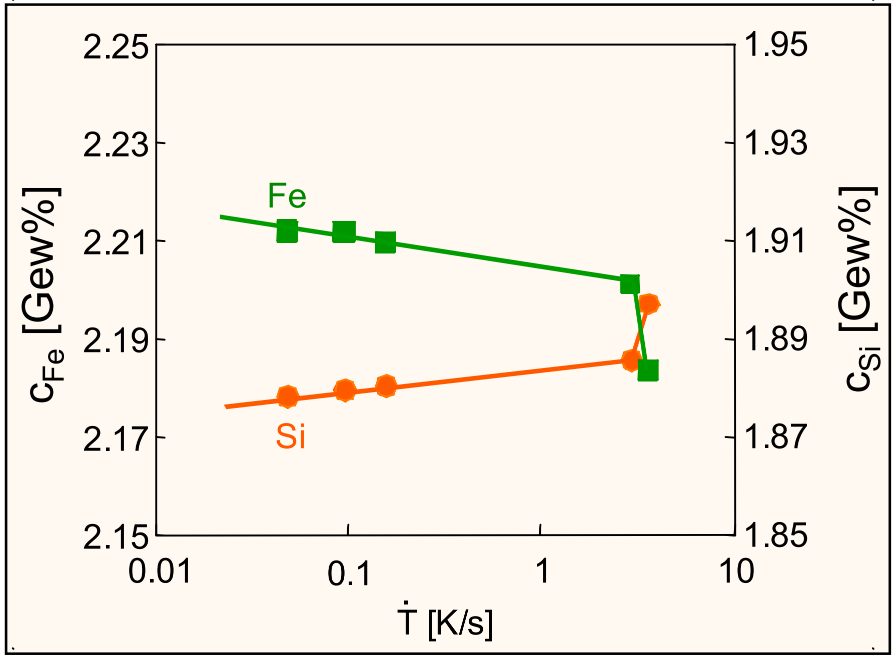






experiment and simulation





reliable phase diagrams are a prerequisite for solidification simulation

kinetic calculations are not meaningful if phase diagram is not accurate

technically important features can be modelled

qualitative predictions most important (solidifying phases, solidification path)

quantitative predictions for design of further processing steps

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

Scheil conditions and lever rule do not necessarily represent limiting cases

in ternary or multicomponent alloys