MatCalc
Engineering

Performing Scheil-Gulliver (SG) analysis in MatCalc

(MatCalc 5.62.0013)

P. Warczok

Outline

- Solid phase composition after alloy solidification
- Back-diffusion effect
- Primary precipitates
- Modeling of solid-solid transformation

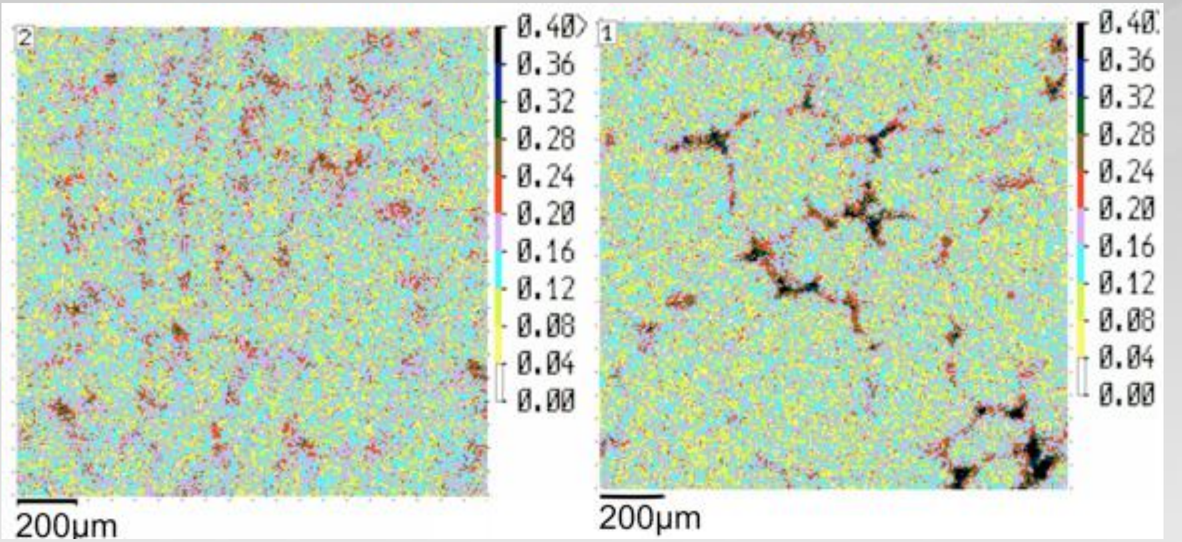
Solid phase composition after alloy solidification

Solid phase composition

- Experimental observation: Microsegregation in solidified phase

Nominal composition of the investigated steel [wt%].

C	Mn	Al	Ti	V	Nb	N
0.21	1.553	0.0249	0.0028	0.137	0.0008	0.0135

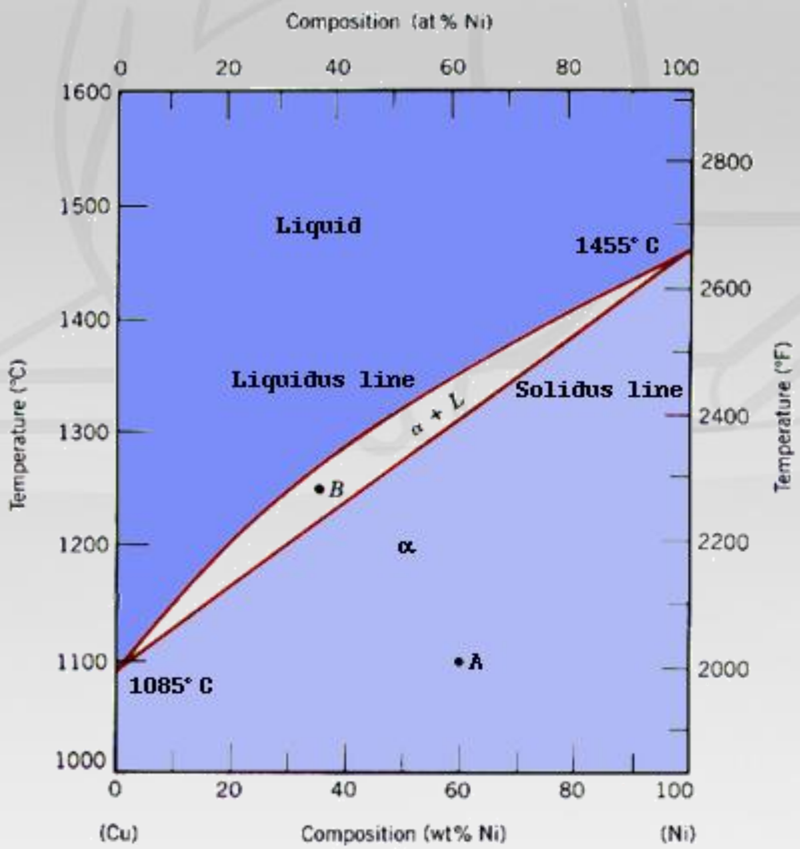


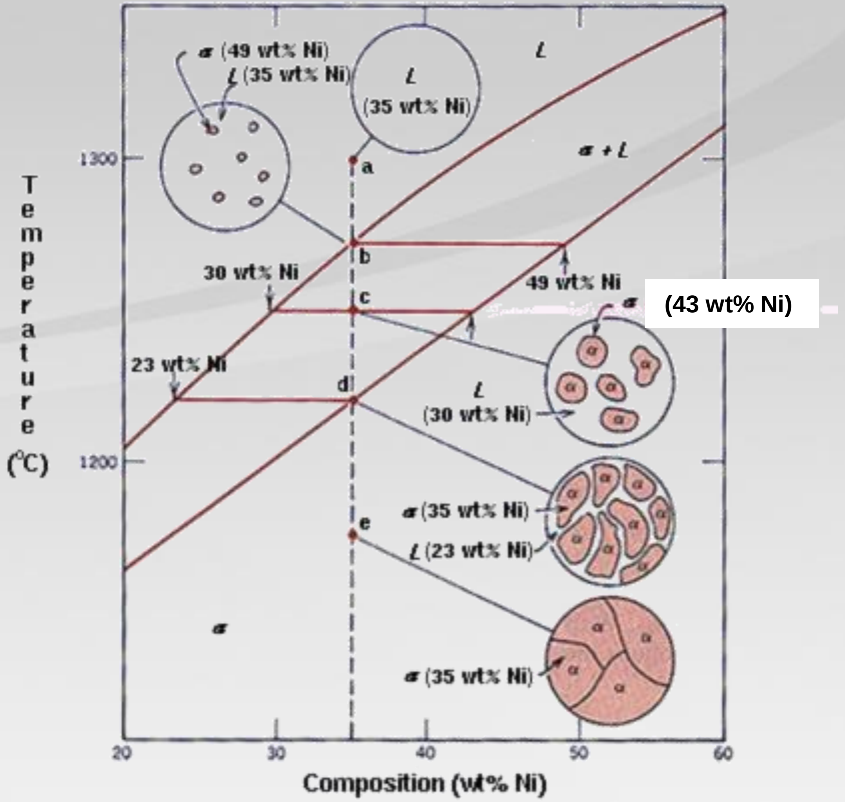
Vanadium concentration (wt.-%) mapping of continuously cast steel: left – region near bloom surface; right – bloom centre.

Pudar M. et al., Steel Res. Int. 81 (2010) 372-80

Solid phase composition

- Theoretical estimation: equilibrium diagram

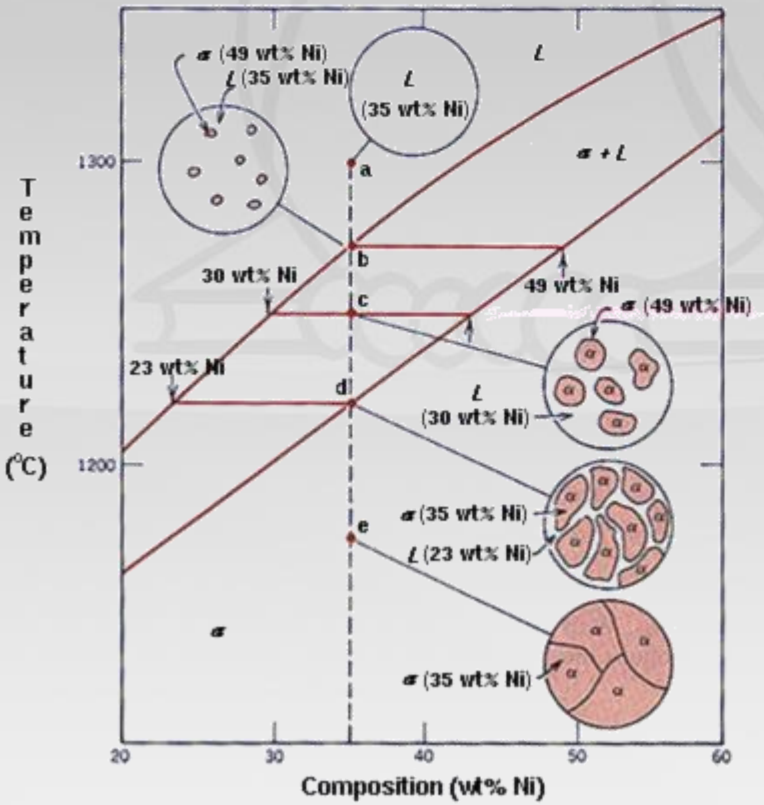




http://www.sv.vt.edu/classes/MSE2094_NoteBook/96ClassProj/examples/cu-ni.html

Solid phase composition

- Theoretical estimation: equilibrium diagram



Are these phase compositions real?

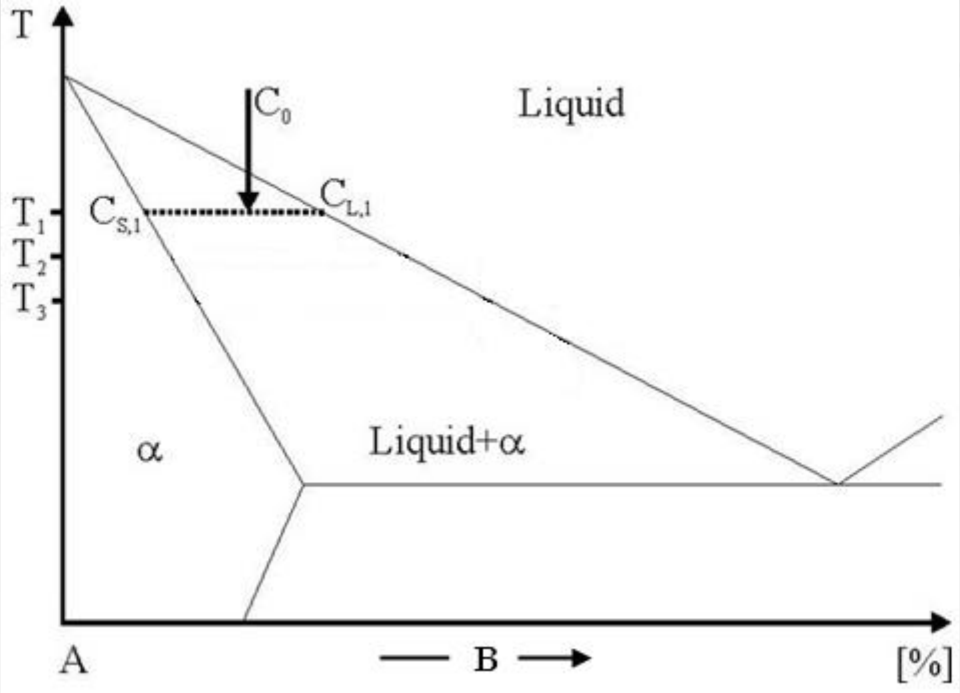
Yes, if diffusion in the phases is fast enough…

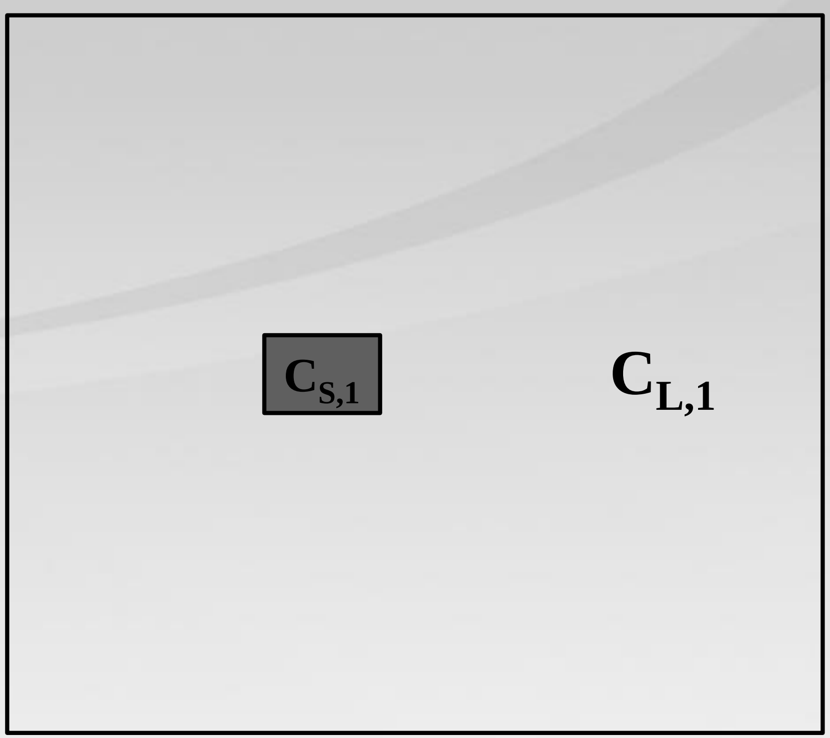
Diffusion in the solid phase is the limiting parameter

http://www.sv.vt.edu/classes/MSE2094_NoteBook/96ClassProj/examples/cu-ni.html

Solid phase composition

- Theoretical estimation: stepped solidification





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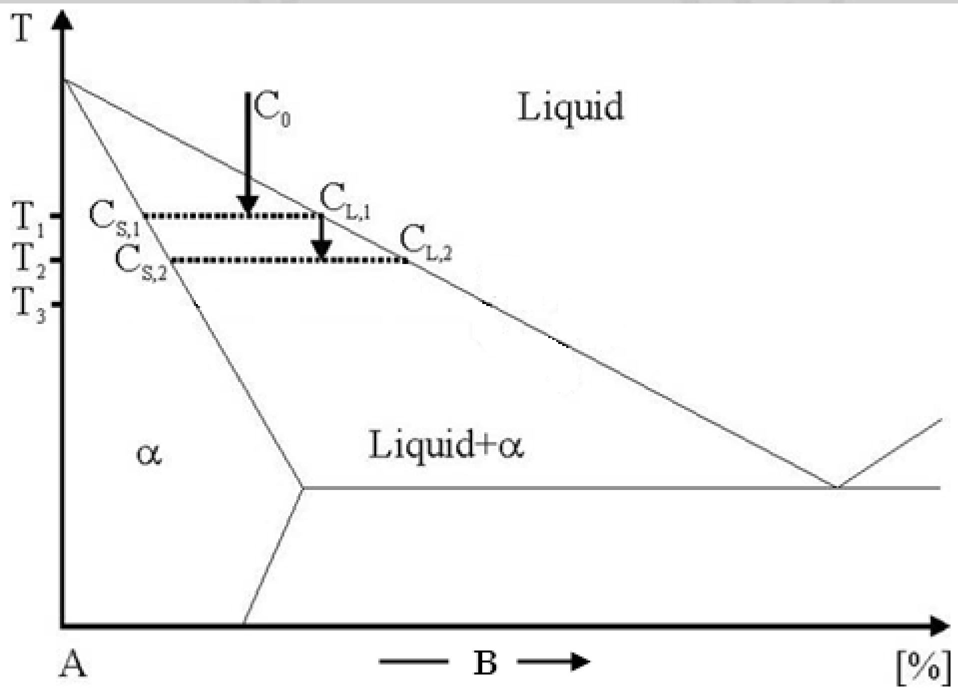
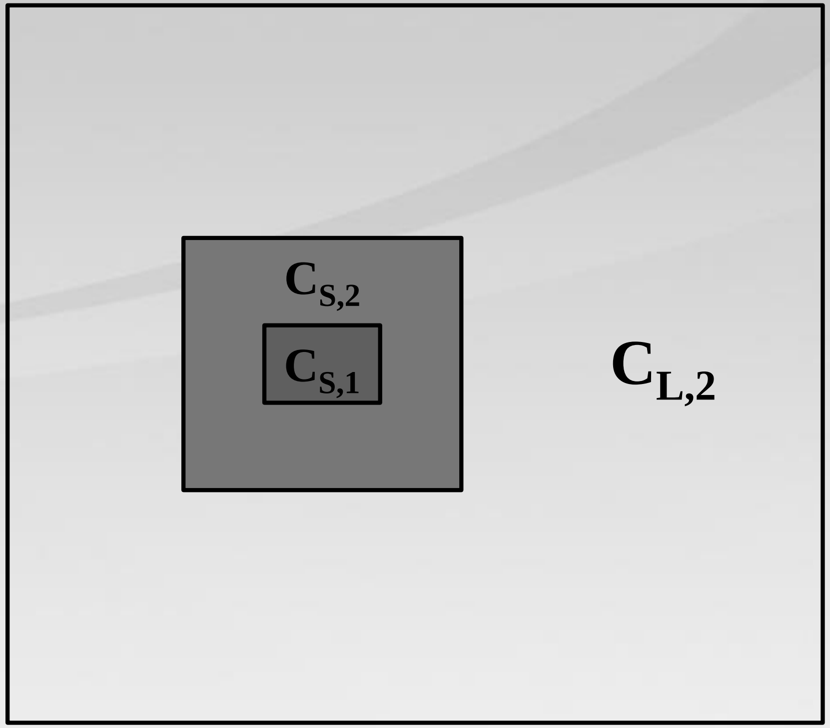
Solid phase composition

• Theoretical estimation: stepped solidification





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Solid phase composition

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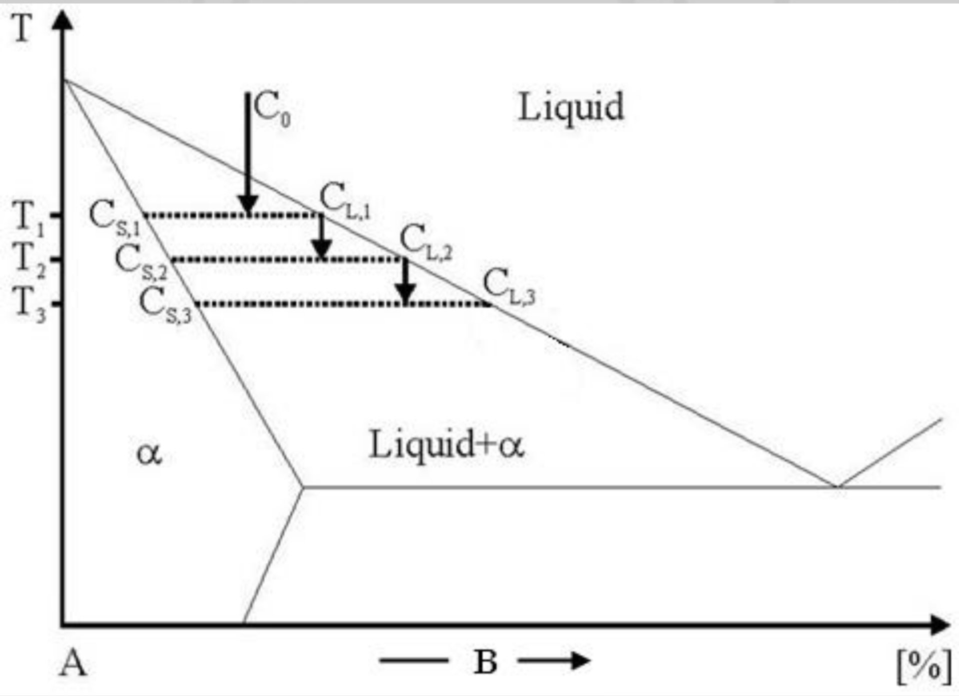

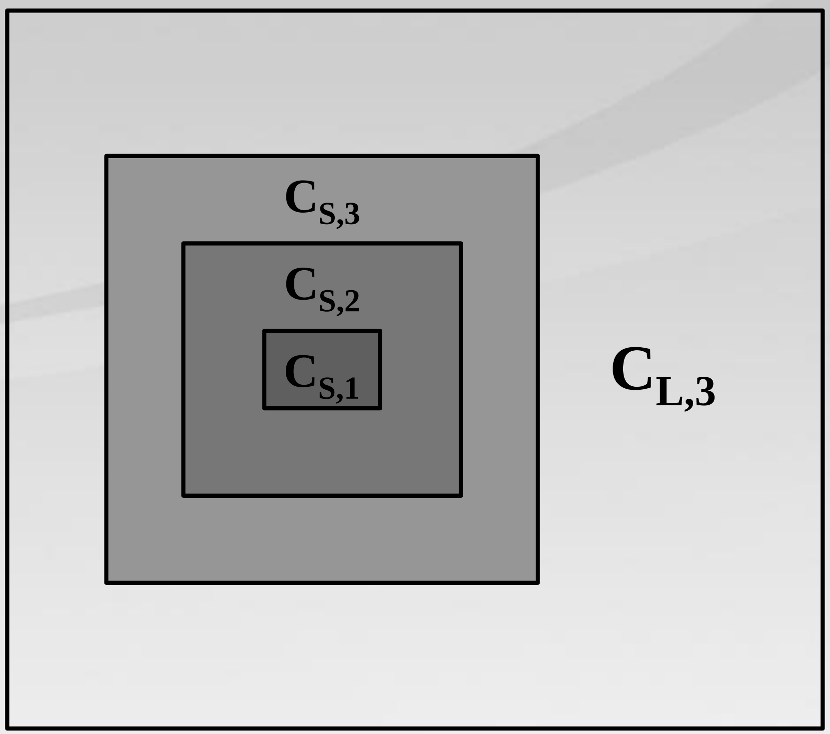

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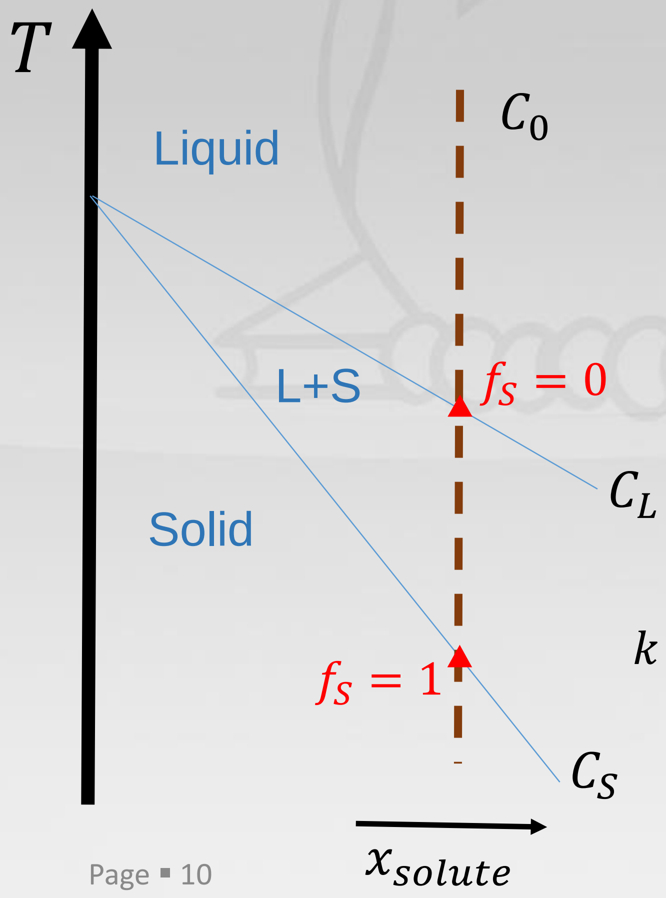
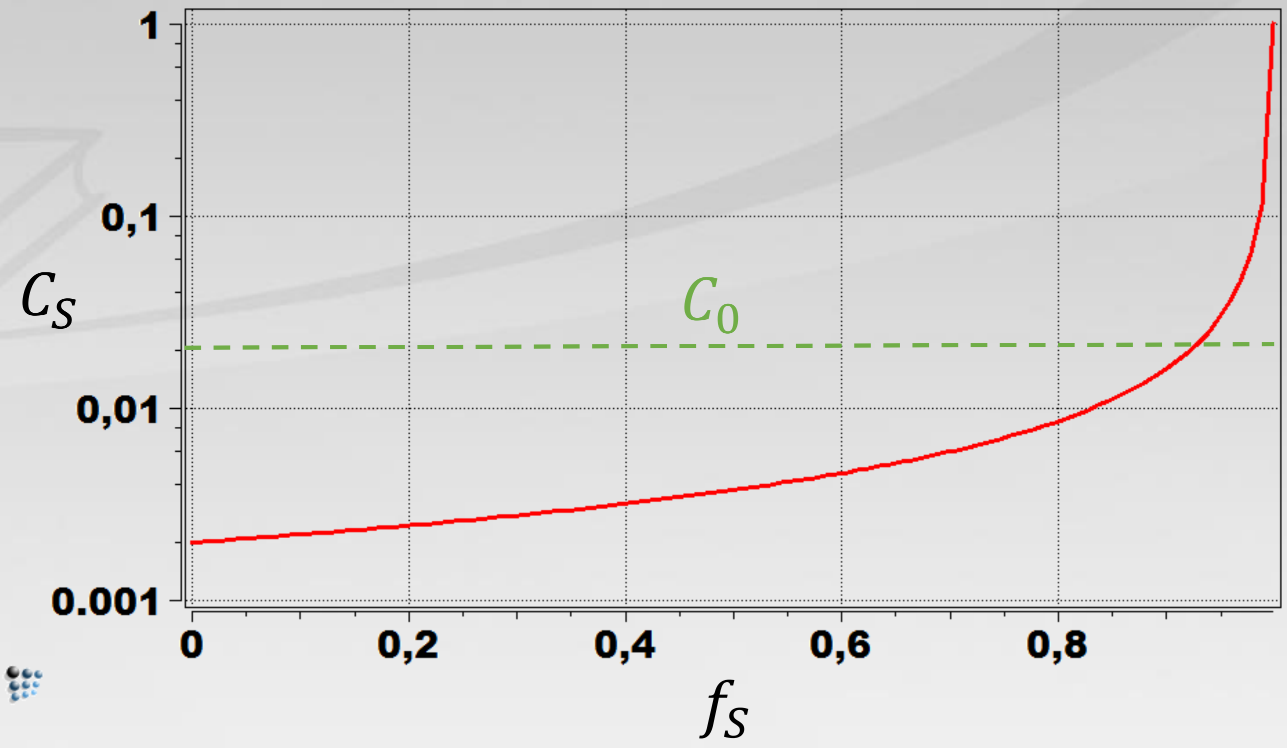
Solid phase composition

- Theoretical estimation: Scheil equation

$$C_S = kC_0(1-f_S)^{k-1}$$



$$k = \frac{C_S}{C_L}$$



Gulliver G.H., J. Inst. Met. 9 (1913) 120-54

Scheil E., Z. Metall. 34 (1942) 70-72

Solid phase composition

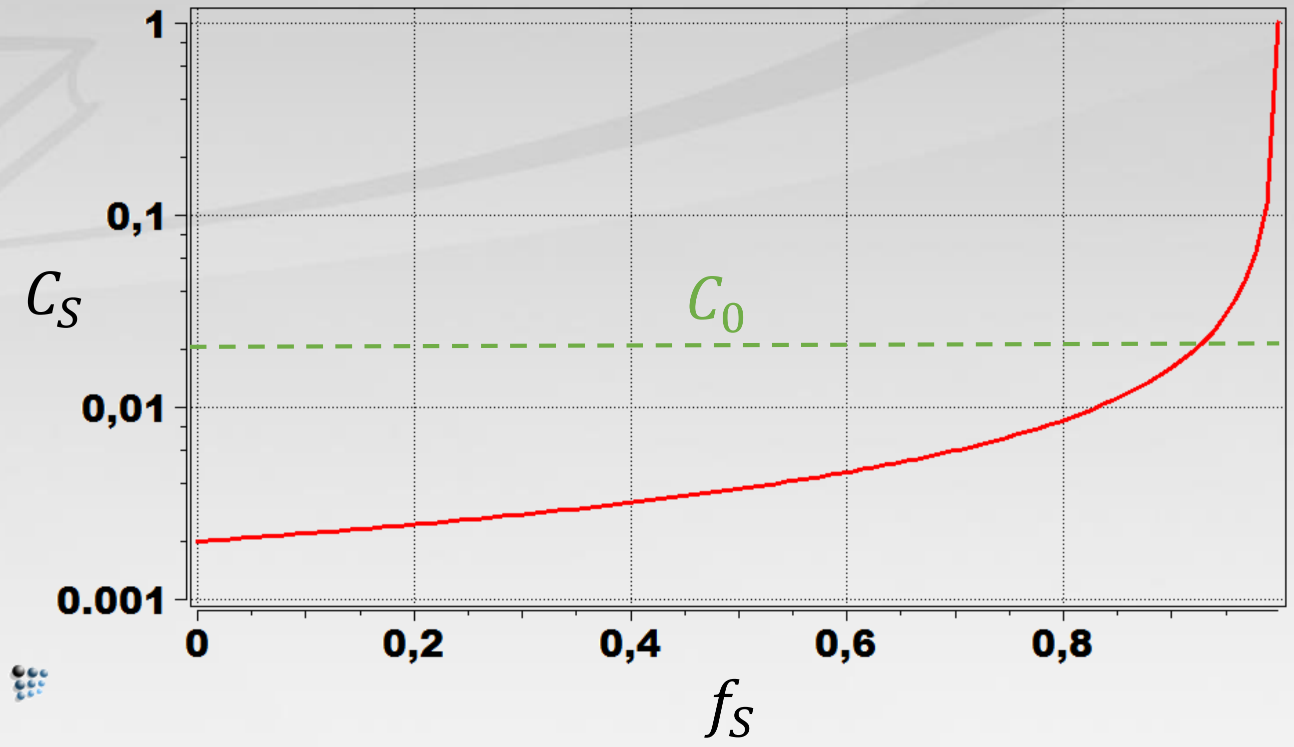
- Theoretical estimation: Scheil equation

Valid for k = const. !

$$C_S = kC_0(1 - f_S)^{k-1}$$

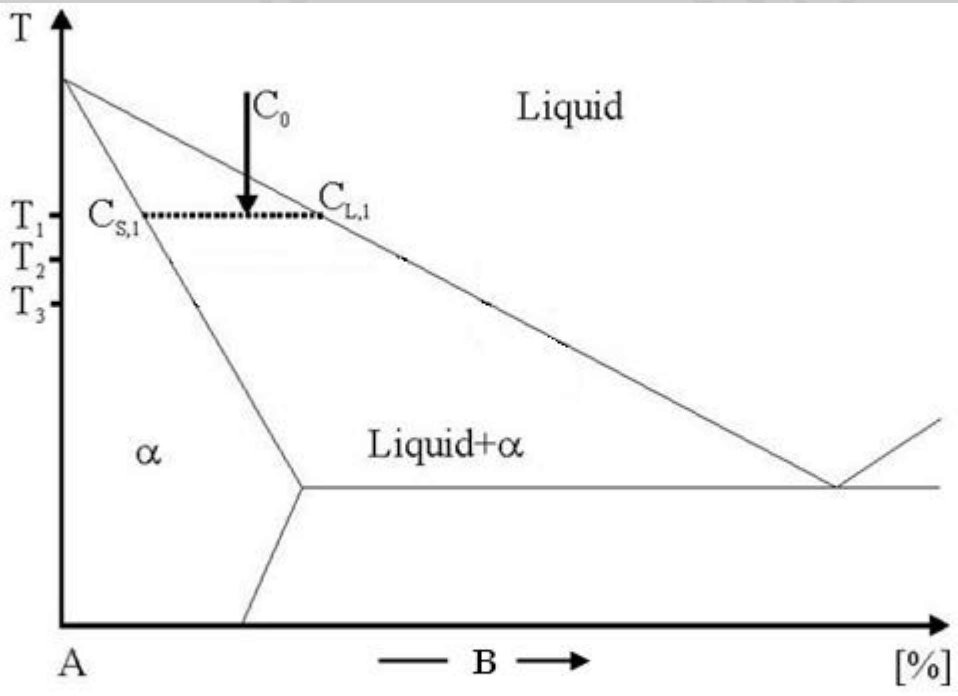
Pro: Nice analytical solution

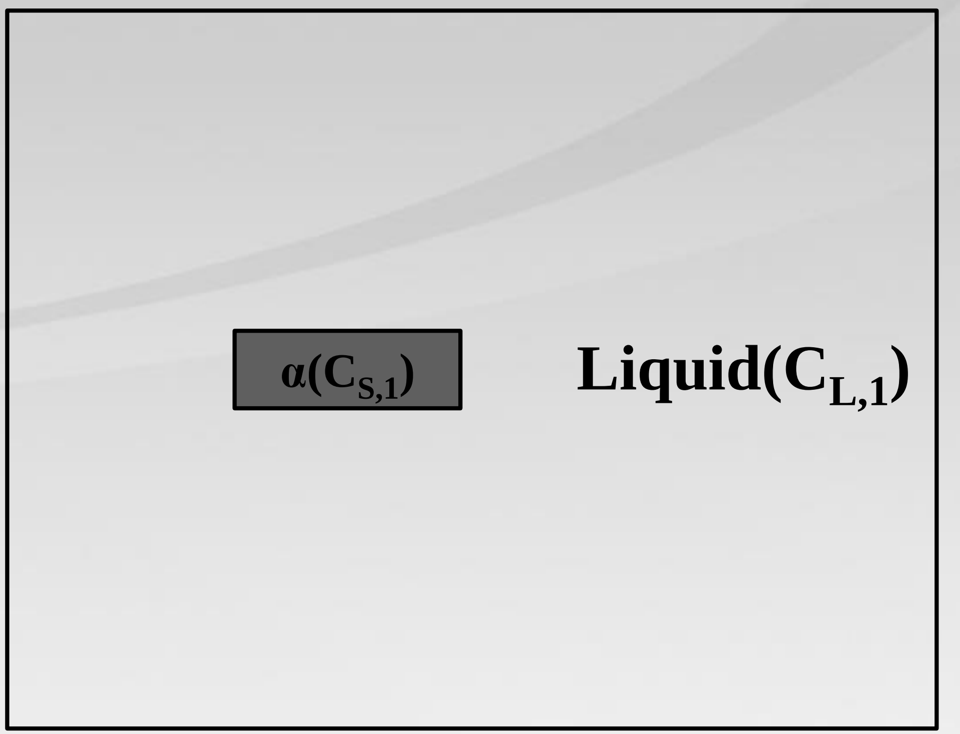
Contra: Formula dependent on system specification



What MatCalc does?

- Stepped solidification → SG-calculation





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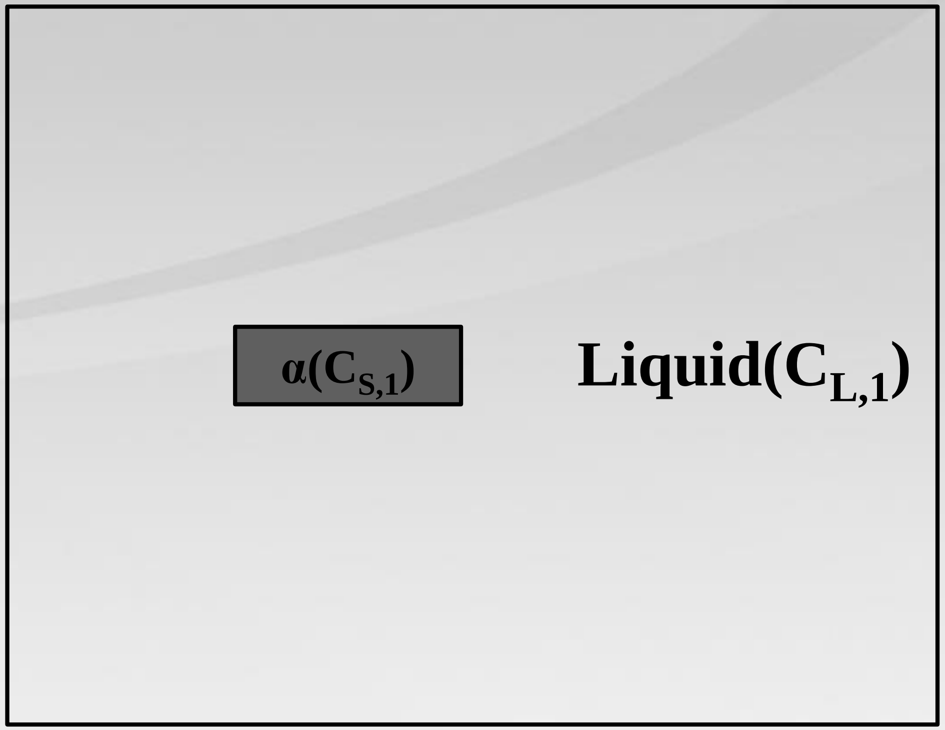
What MatCalc does?

- New equilibrium phase α with solute content $C_{S,1}$ created
- Liquid composition set to $C_{L,1}$



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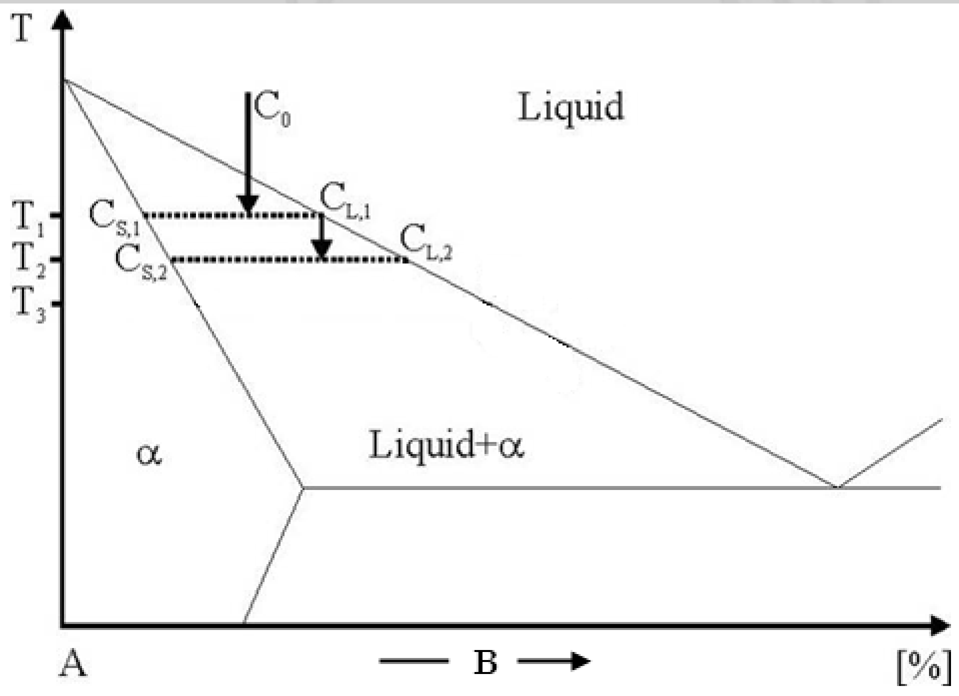

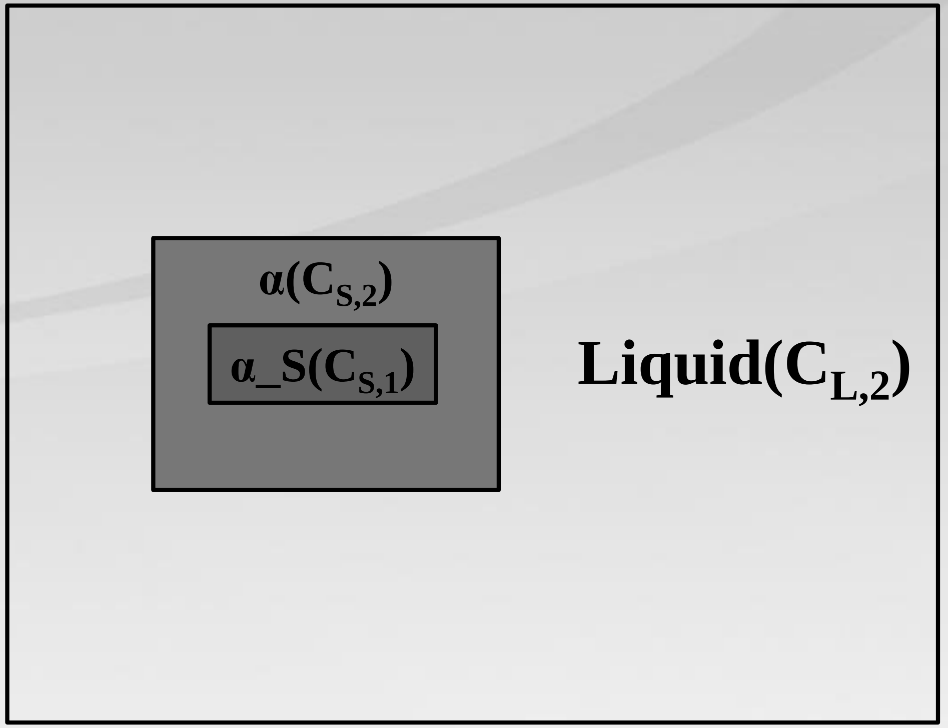

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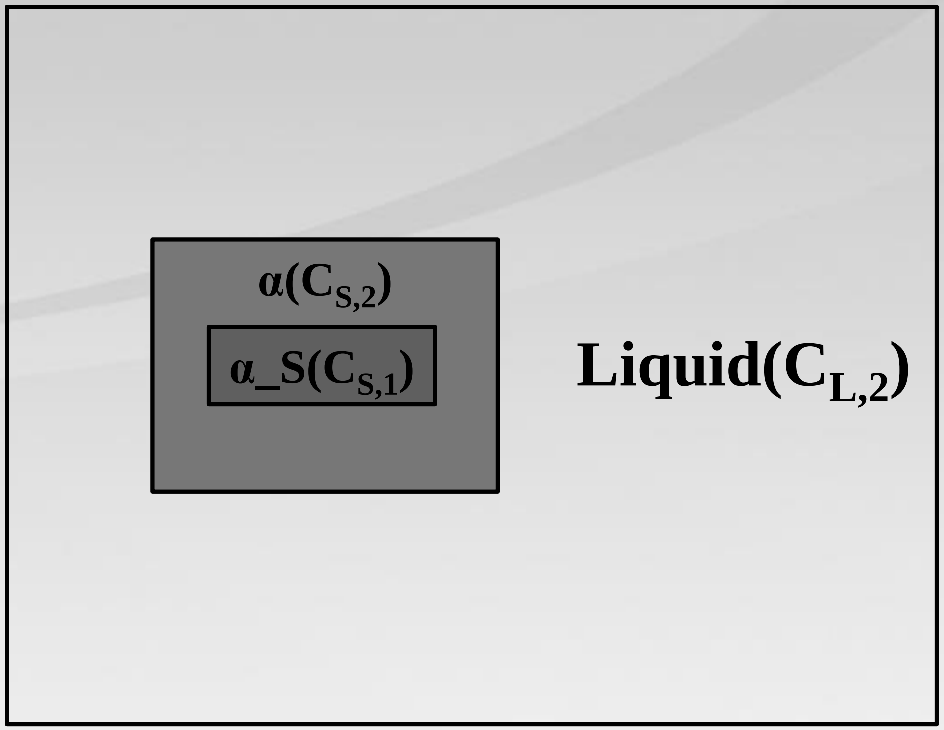
What MatCalc does?

- Previous α-phase is denoted now α_S
- α_S gets a „dormant" status (phase fraction and composition are „frozen")
- New equilib. phase α with solute content $C_{S,2}$ created
- Liquid composition set to $C_{L,2}$



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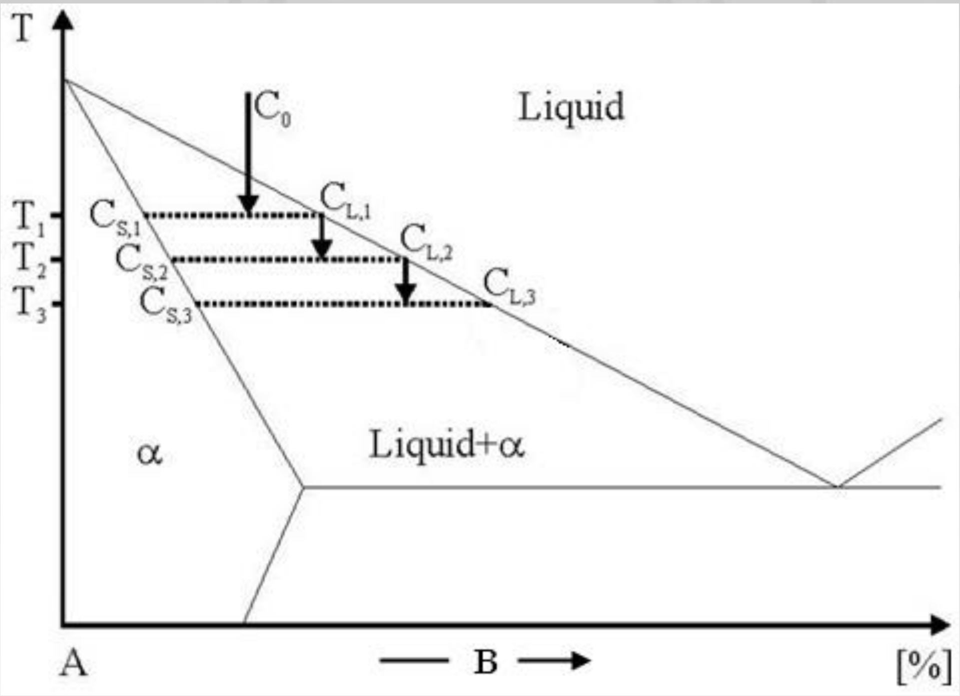
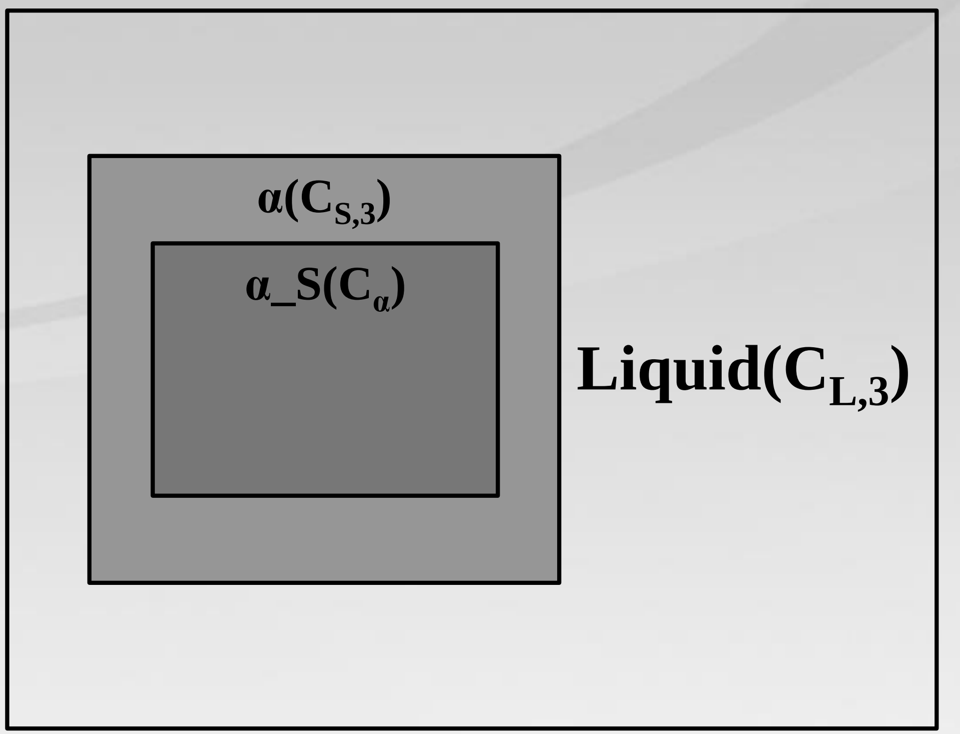
What MatCalc does?





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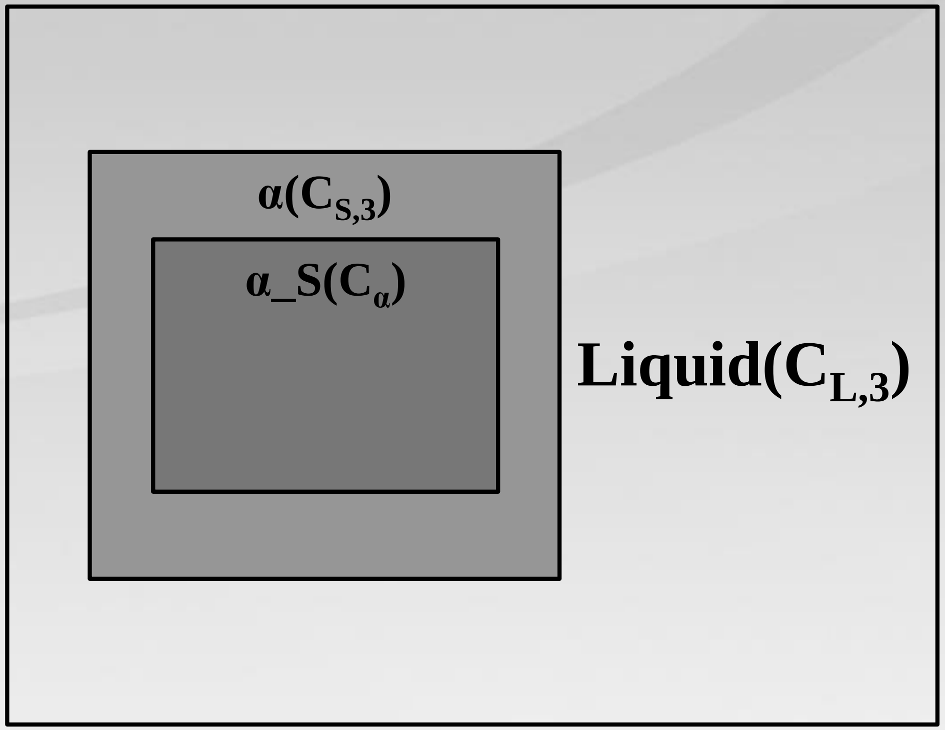
What MatCalc does?

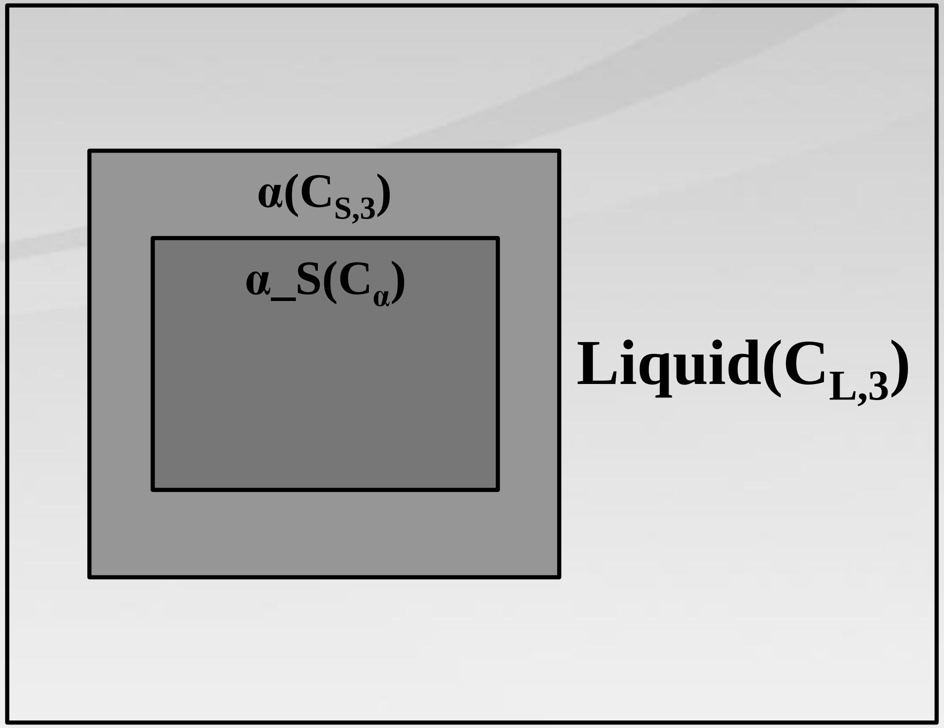
- α_S formed by merging the previous α_S and previous α (adding phase fractions)
- α_S composition is evaluated from mass balance of the merged phases
- „Dormant“ status set to α_S
- New equilib. phase α with solute content $C_{S,3}$ created
- Liquid composition set to $C_{L,3}$



What MatCalc does?

Technical note

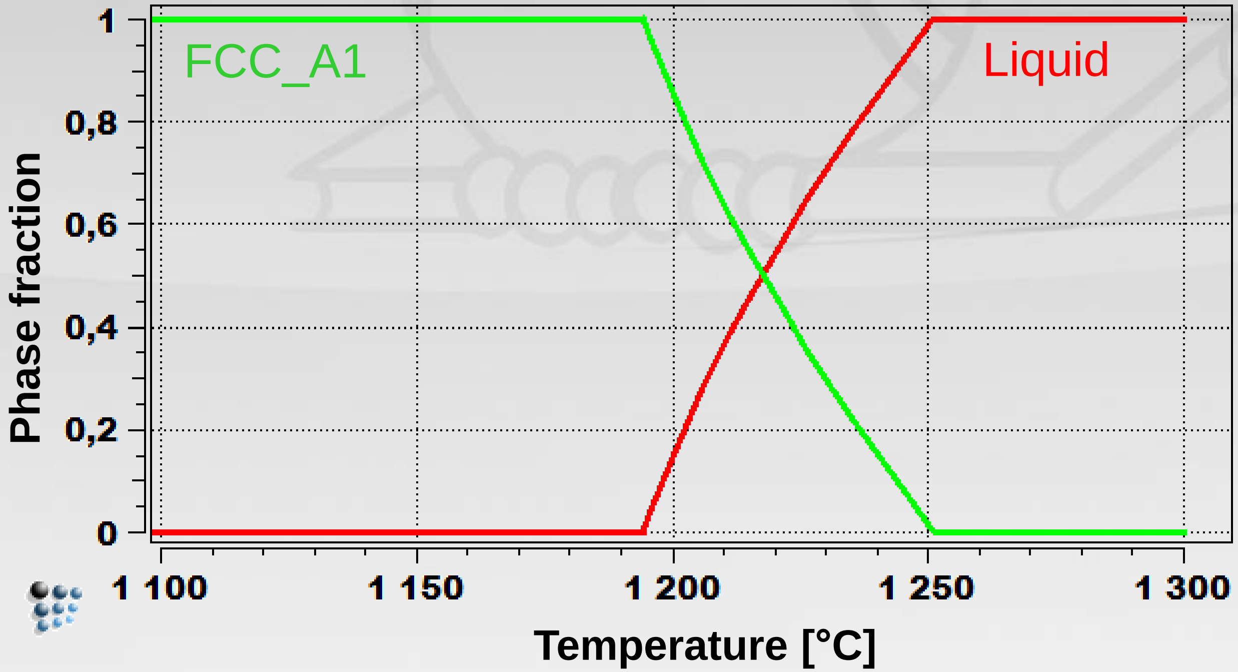
- „α"-phase contains the fraction solidified **at** the considered temperature
- „α_S"-phase contains all fractions solidified **before** the considered temperature



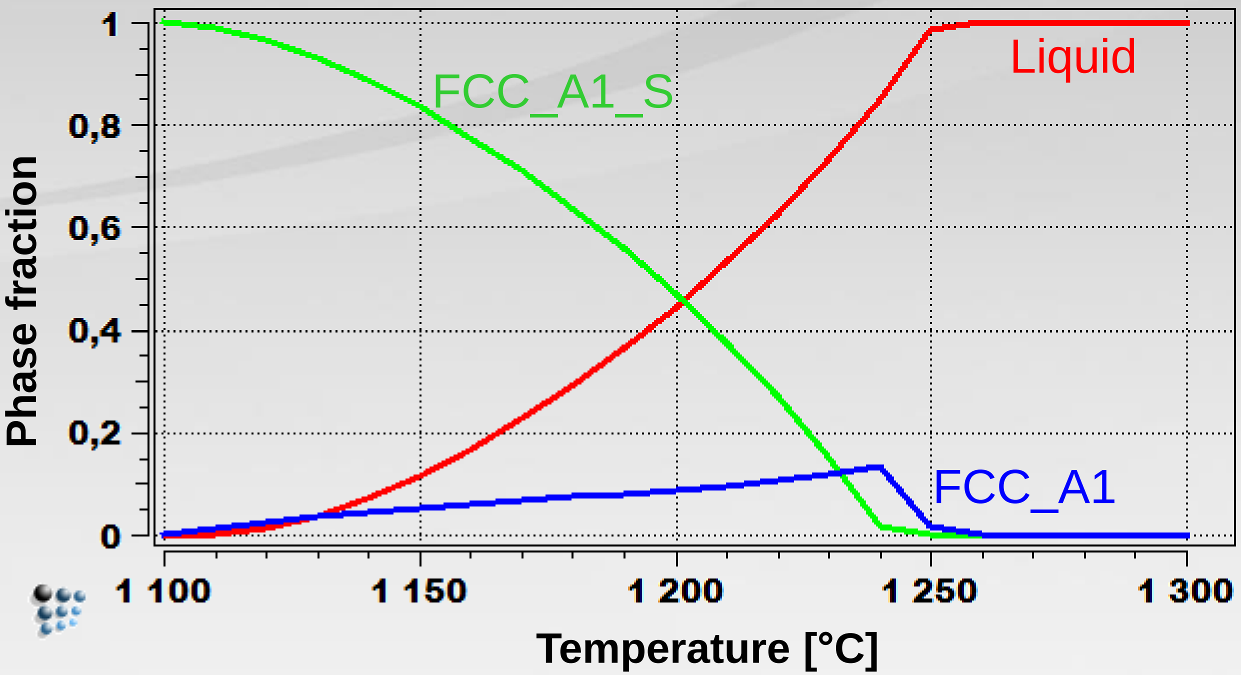
Example

- Cu-Ni alloy, 35 wt.% Ni

Equilibrium calculation



SG-calculation



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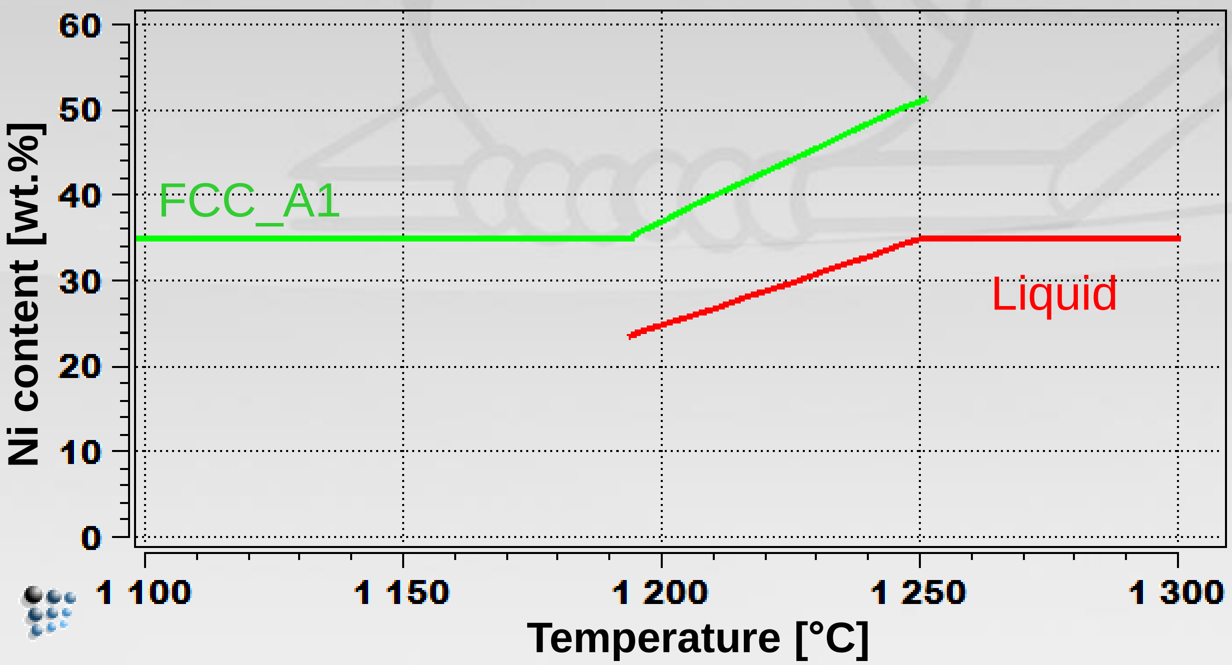
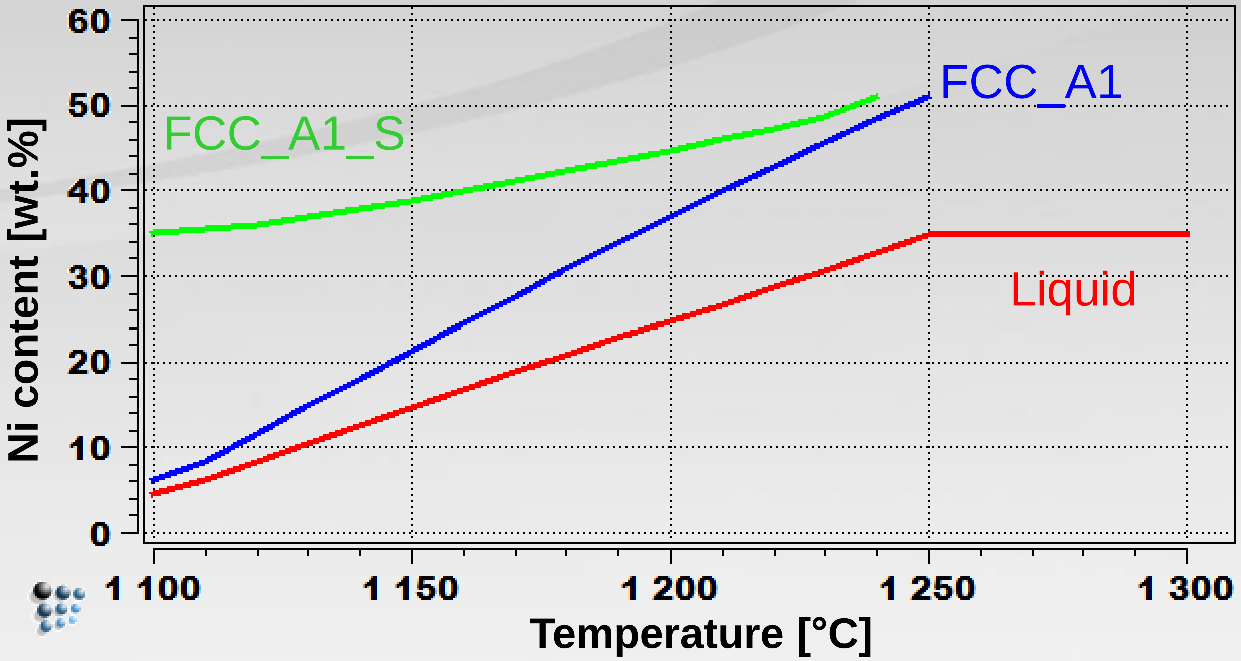


SG-calculation

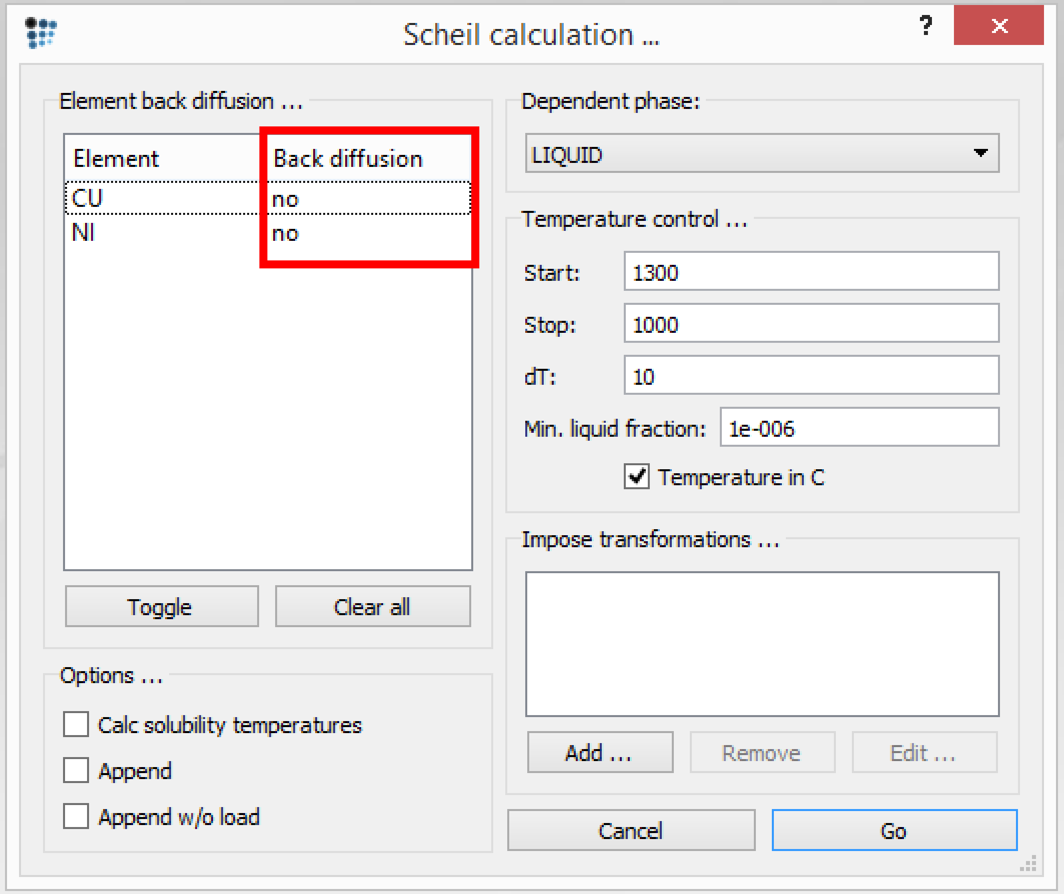


Back-diffusion effect

Backdiffusion

- Some elements might be permitted to equilibrate fast between the liquid and solid phases

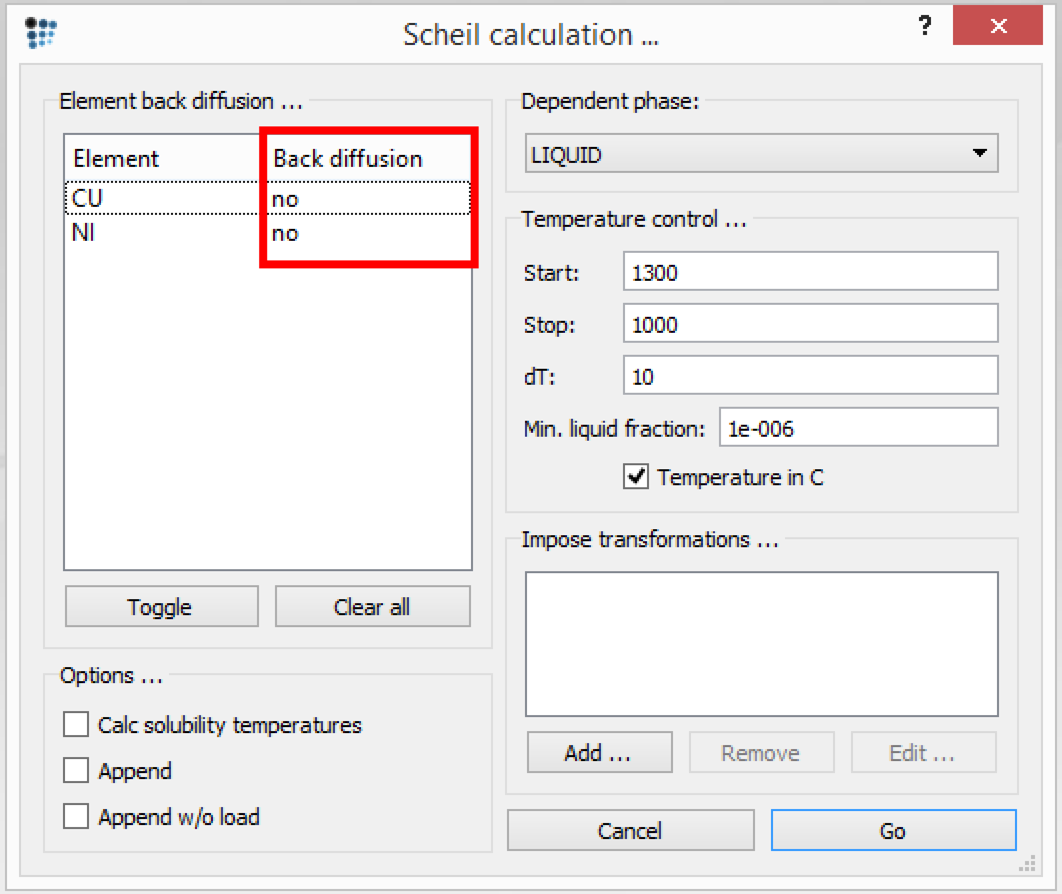
- Relevant for interstitial elements (B,C,N) → diffuse fast enough on the interstitial lattice



Backdiffusion

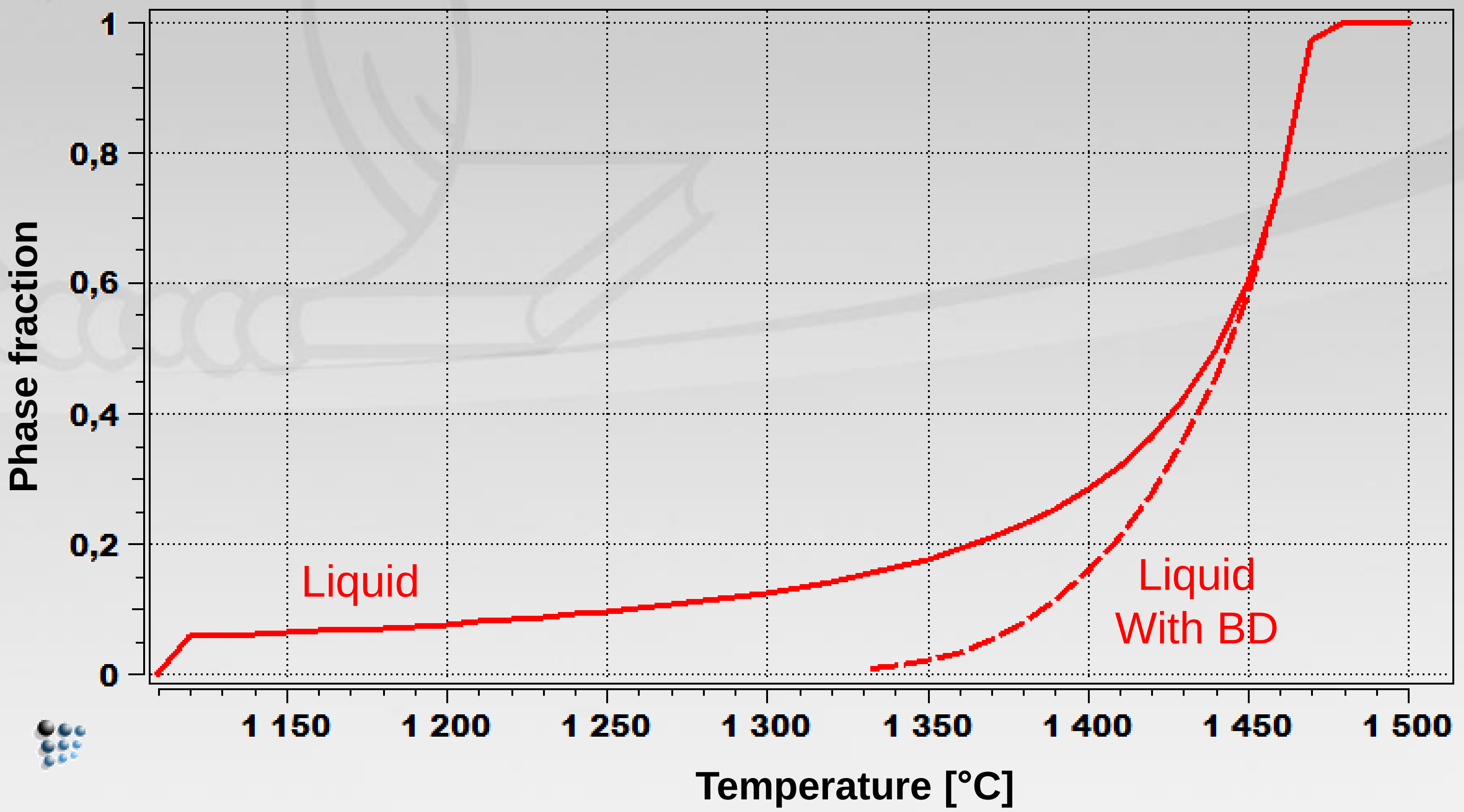
Technical note

„_S“-phase has a „fixed phase fraction flag“ and constraints on u-fraction of elements with „no“ setting for back-diffusion (it is not „dormant“ any more)



Example

- Fe-Mn-C alloy, 3 wt.% Mn, 0.7 wt.% C (Tutorial 11)



Example

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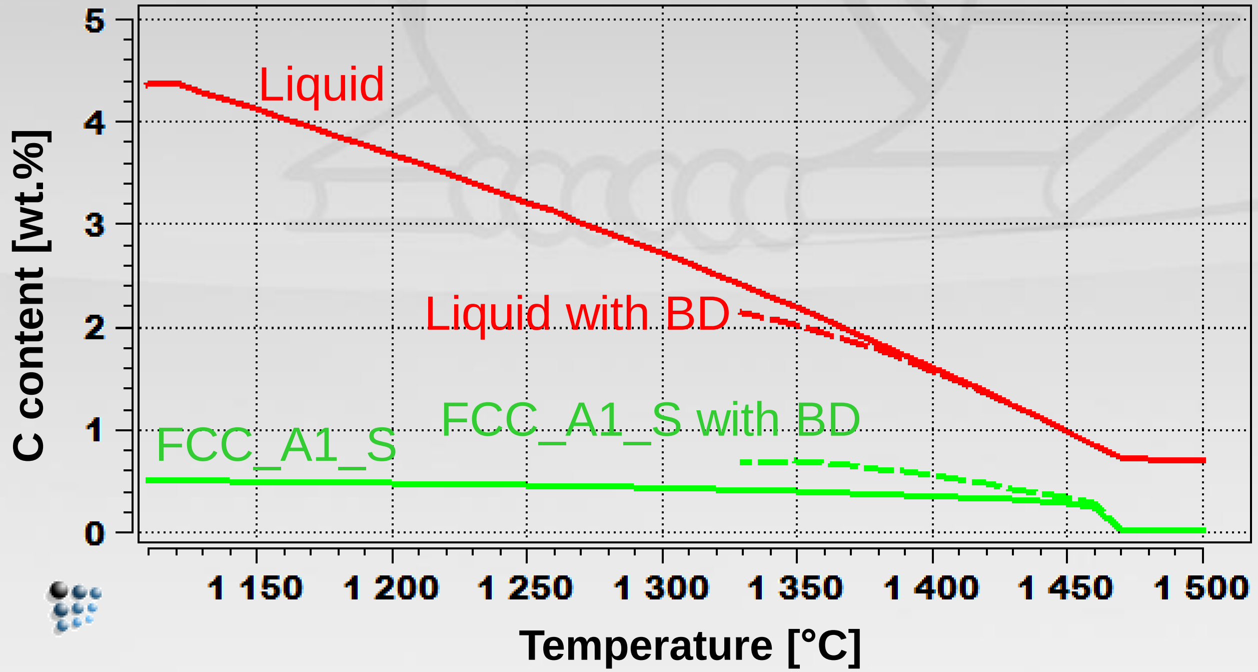
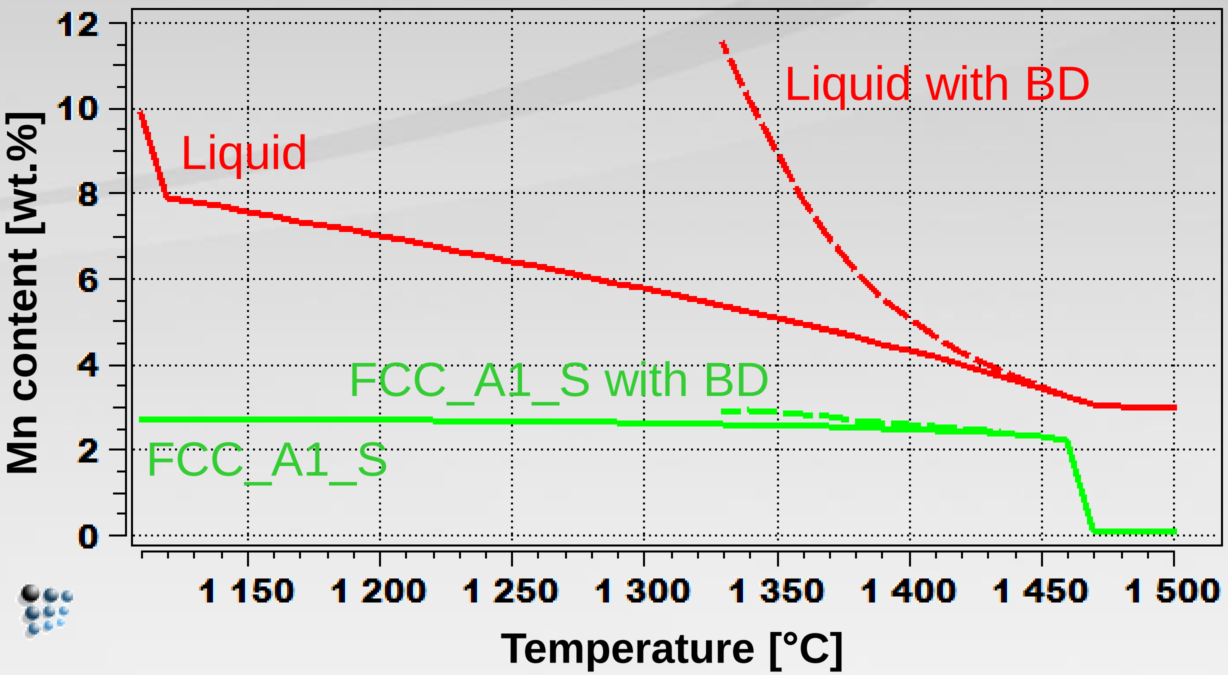


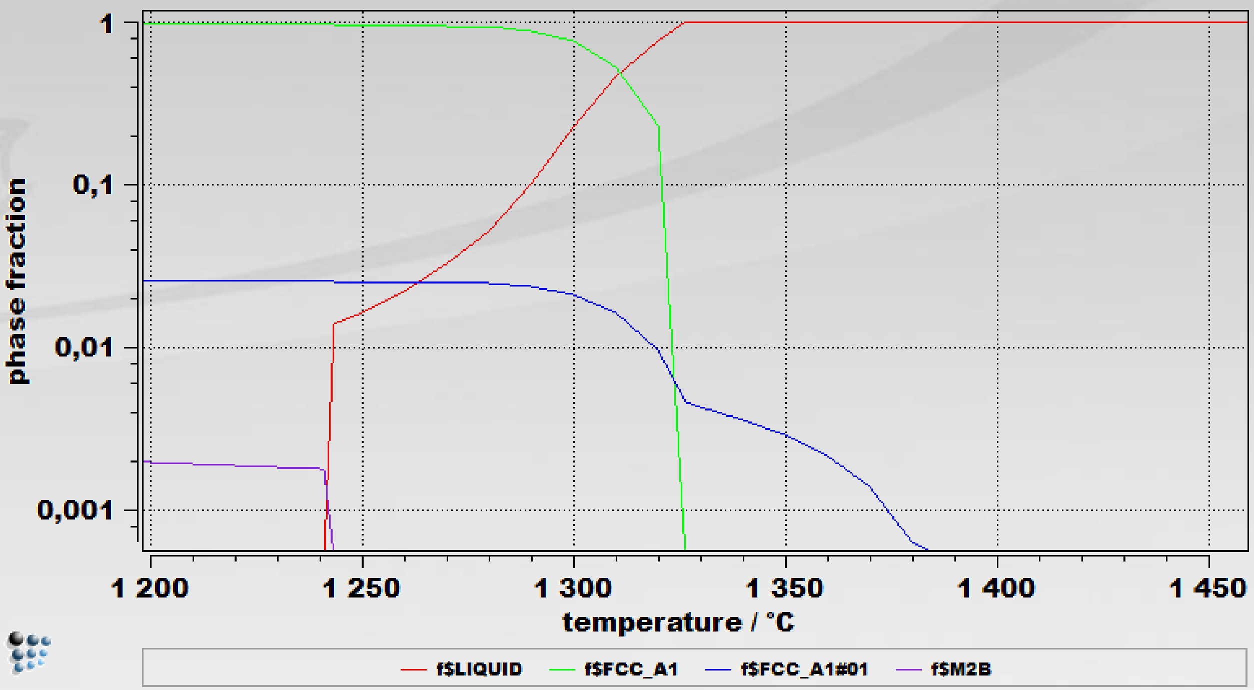


Primary precipitates

Primary precipitates

- Primary precipitates → preciptates formed during the presence of the liquid phase
- Phases coexistent with the liquid phase at the equilibrium calculation → strong candidates for the primary precipitates

Ni-Cr-Mo-Ti-B-C (0.25 wt.% C)

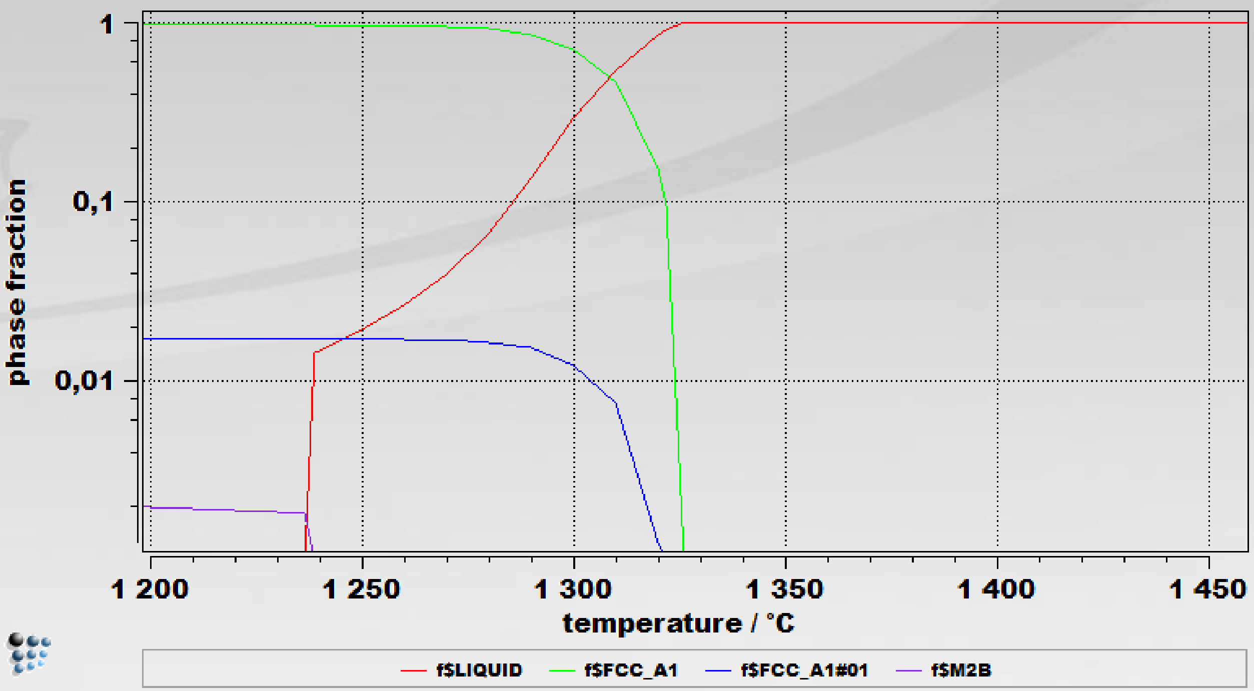


Equilibrium calculation

Primary precipitates

- Primary precipitates are preciptates formed during the presence of the liquid phase
- Phases coexistent with the liquid phase at the equilibrium calculation are strong candidates for the primary precipitates

Ni-Cr-Mo-Ti-B-C (0.1 wt.% C)

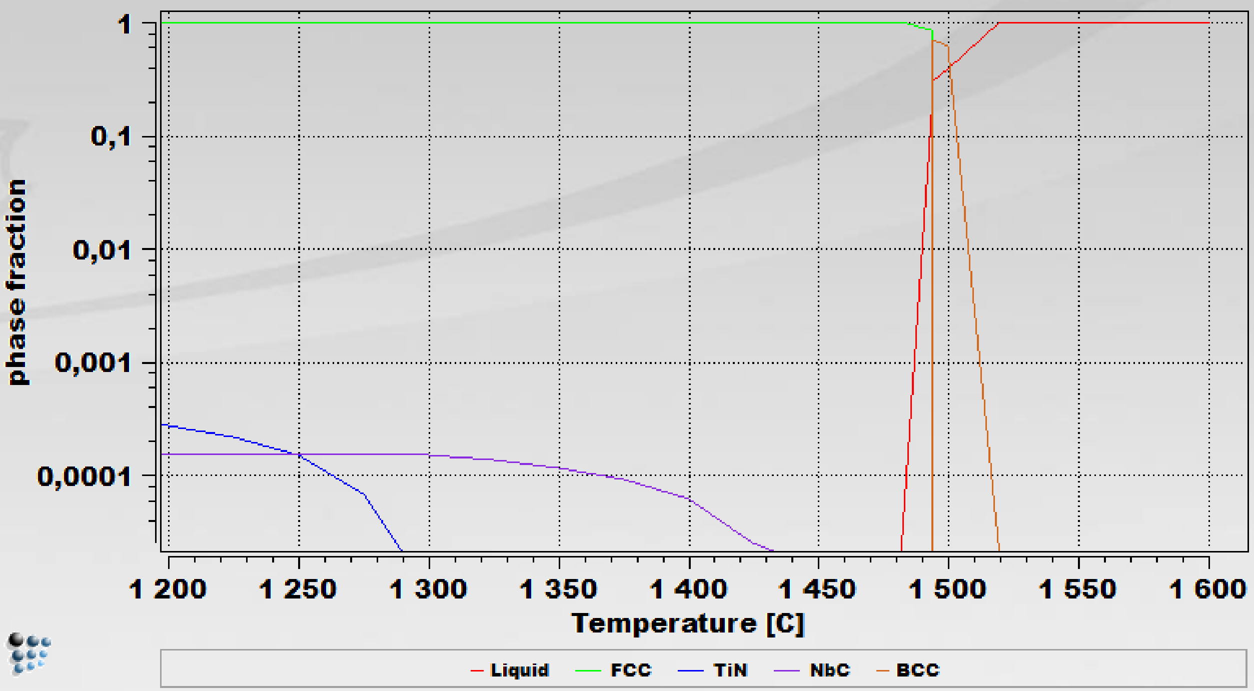


Equilibrium calculation

Primary precipitates

- Primary precipitates are preciptates formed during the presence of the liquid phase
- Phases coexistent with the liquid phase at the equilibrium calculation are strong candidates for the primary precipitates
- Phases appearing close to the liquidus should be also checked

Fe-Nb-Ti-C-N (Example E20)



Equilibrium calculation

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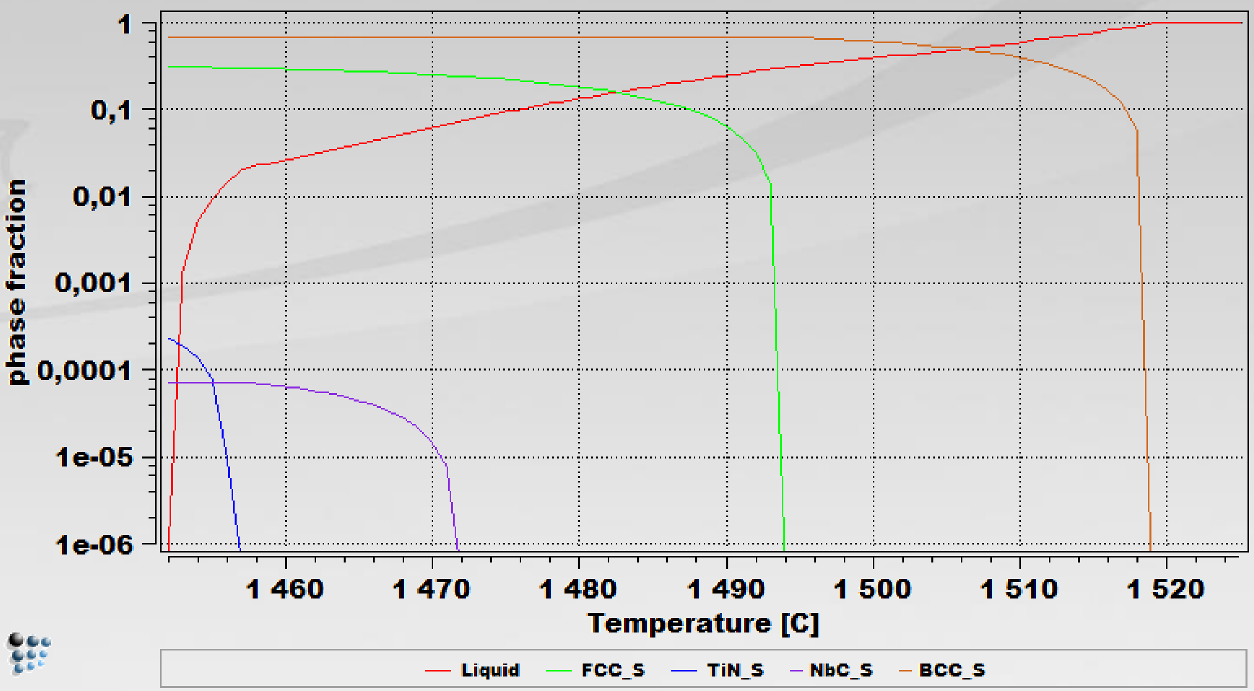

SG-calculation

Modeling of solid-solid transformation

Solid-solid transformation

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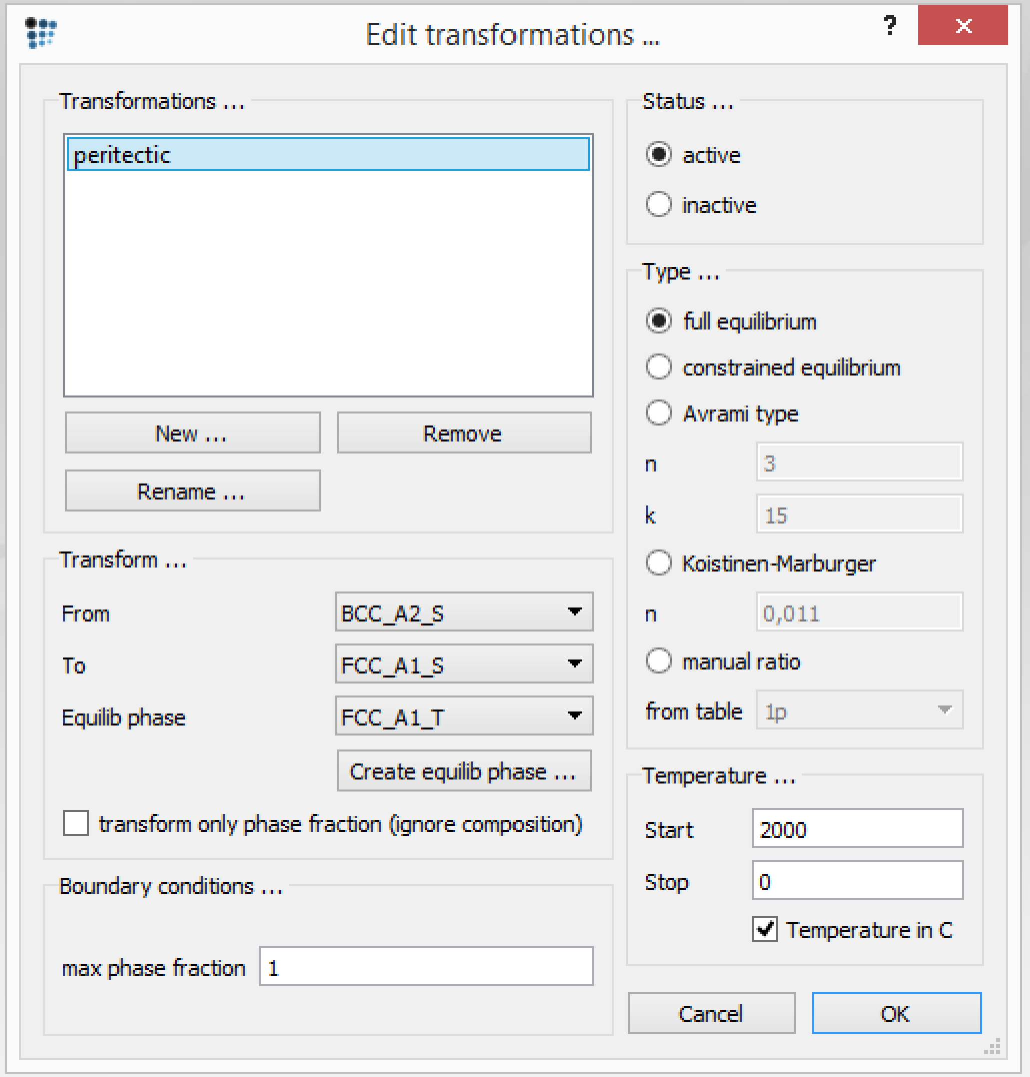
- A solid phase might transform to another solid phase
- Relevant for the peritectic reaction (e.g. δ-ferrite + liquid → austenite in steels)



Solid-solid transformation

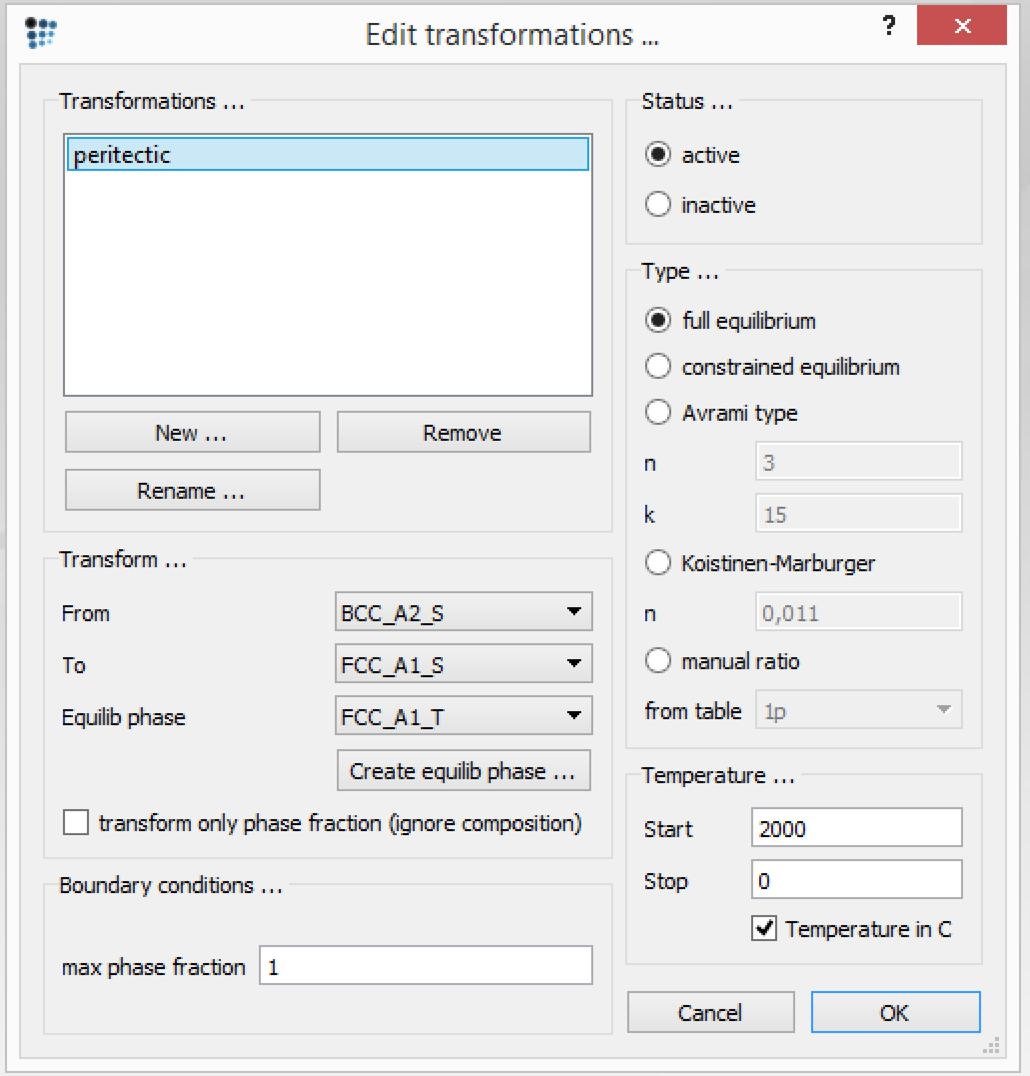
- Transformation type (calculation of the transformed phase ratio)
  - Full equilibrium
  - Constrained equilibrium
    - As „full“, but the back-diffusion constraints are taken into account
  - Avrami type

$$f = 1 - exp\left(-kT_{frac}^{n}\right) \qquad T_{frac} = \frac{T - T_{stop}}{T_{start} - T_{stop}}$$

  - Koistinen-Marburger

$$f = 1 - exp\left(-nT_{diff}\right) \qquad T_{diff} = T_{start} - T$$

  - Manual ratio
    - Amounts taken from the table provided by user (Temperature vs. Amount transformed)



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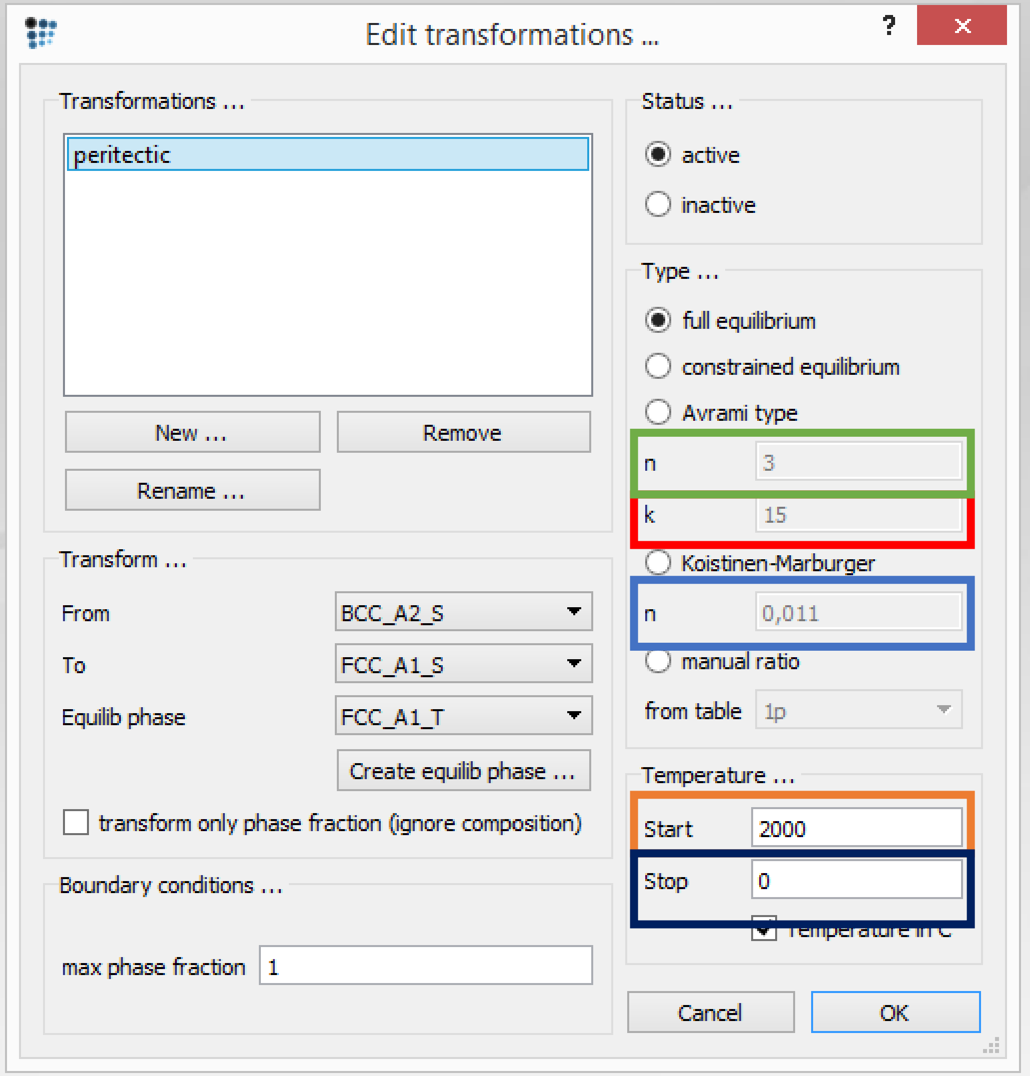
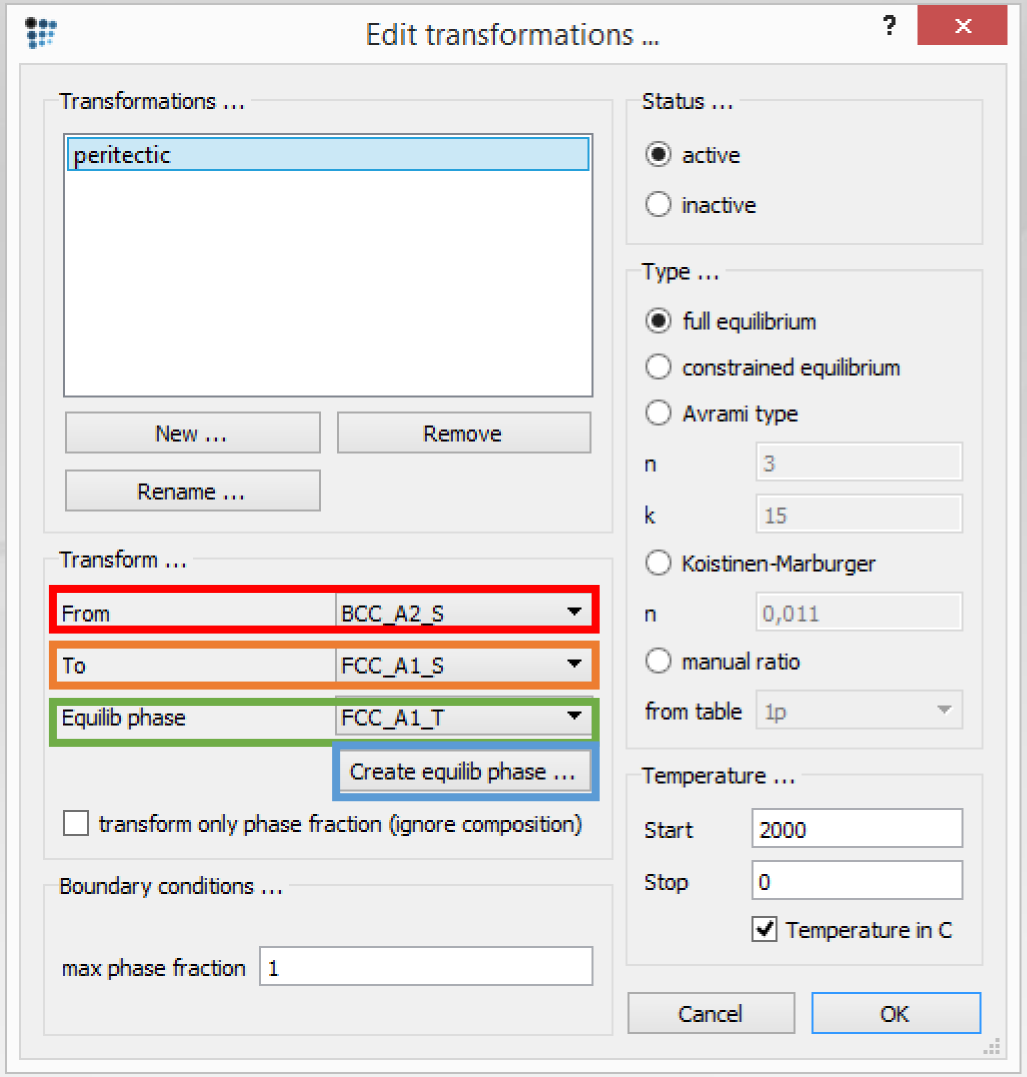


Solid-solid transformation

Technical note

- The „From“-phase is taken and transformed to „Equilib phase“-phase (with „_T“-suffix)
- „Equilib phase“ might be created with „Create equilib phase…“ from parent phase of the „To“-phase
- „_TS“-phase contains all fractions transformed **before and at** the considered temperature



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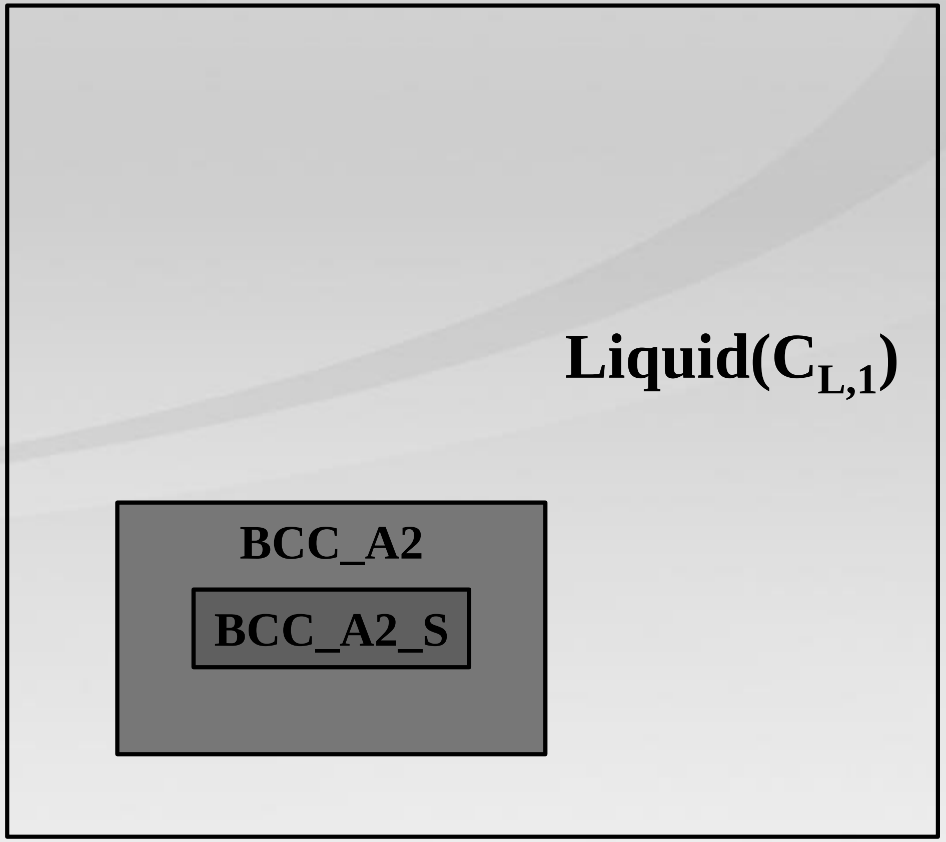

L0 → L1 + BCC_A2

Solid-solid transformation

Technical note

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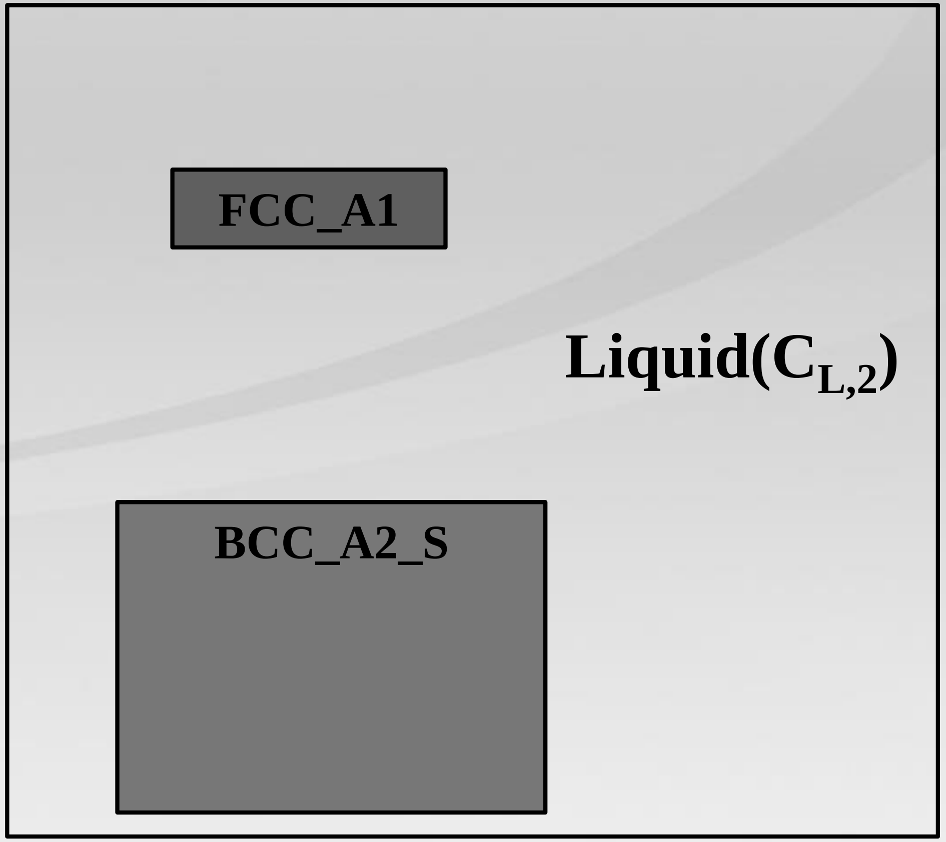

L1 → L2 + FCC_A1

Solid-solid transformation

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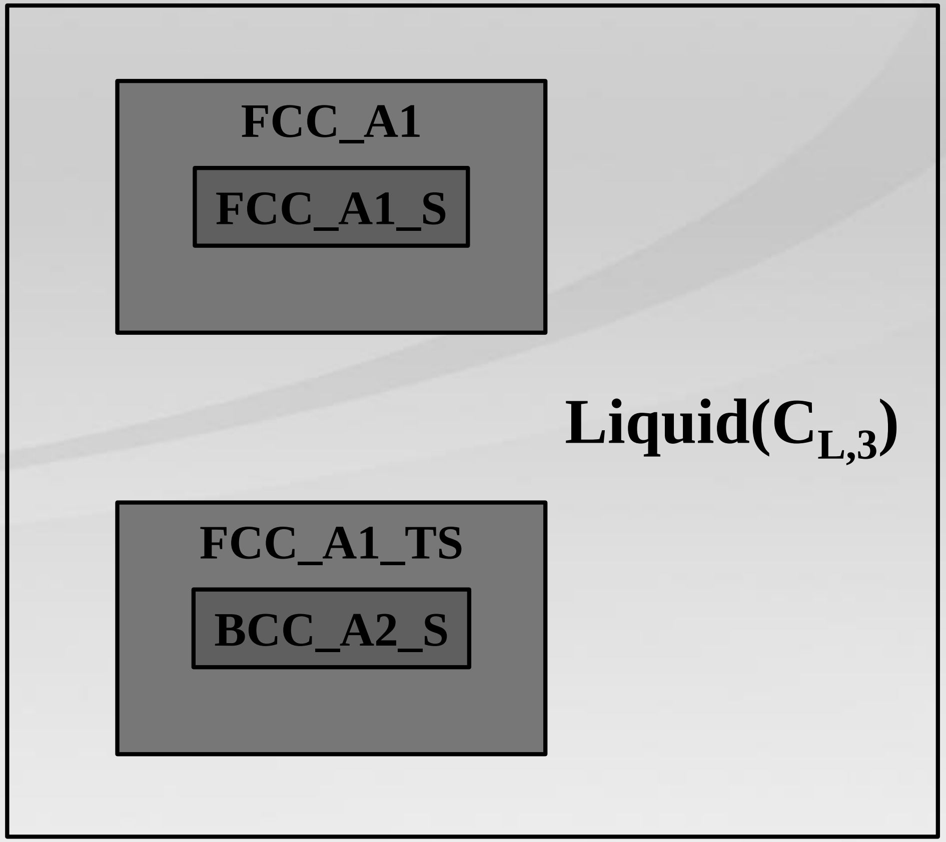
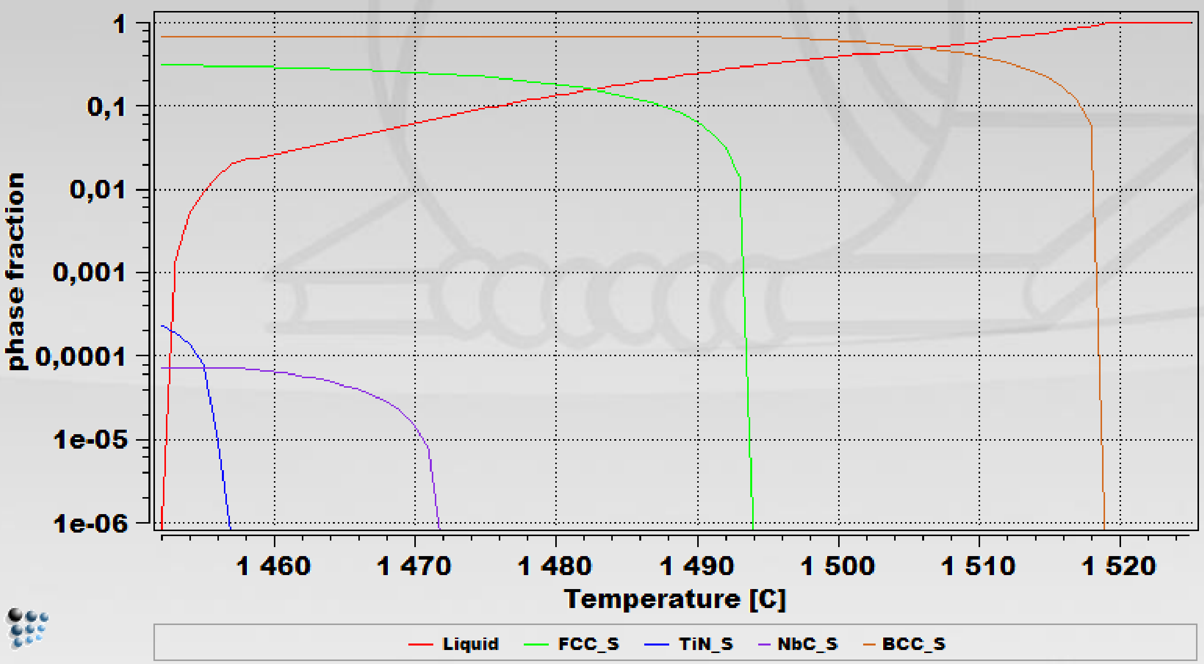


L2 → L3 + FCC_A1

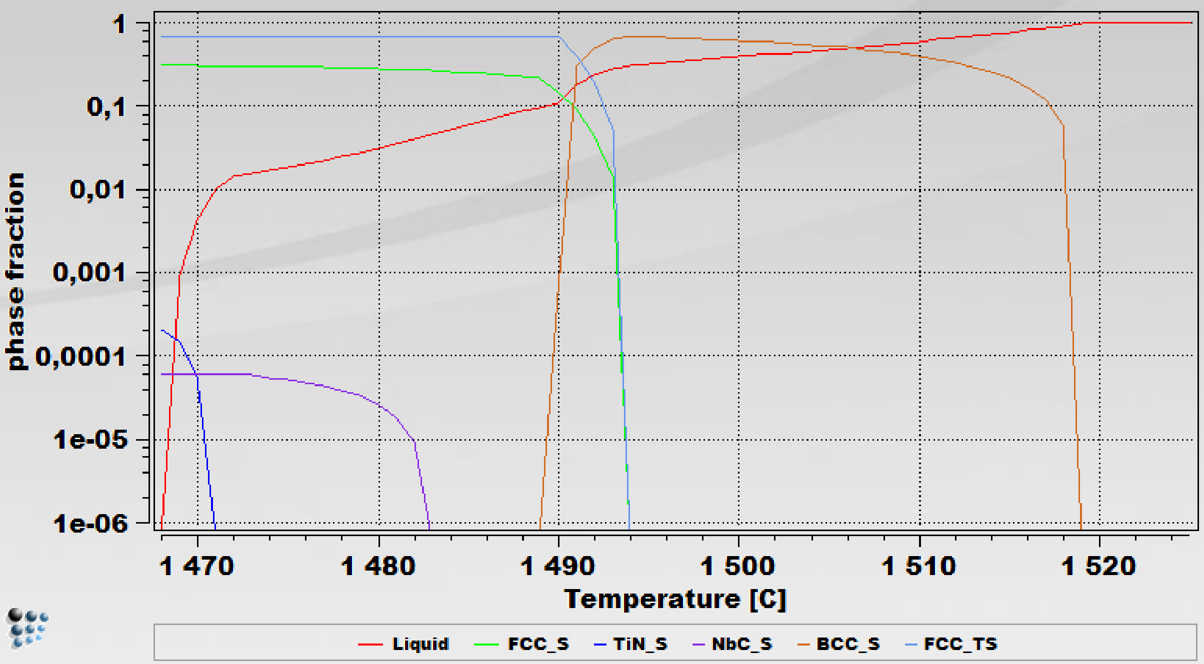
BCC_A2_S + L2 → FCC_A1_TS

Solid-solid transformation

Fe-Nb-Ti-C-N (Example E20)



Without peritectic transformation



With peritectic transformation

Applications

MatCalc Engineering

What do I get from it?

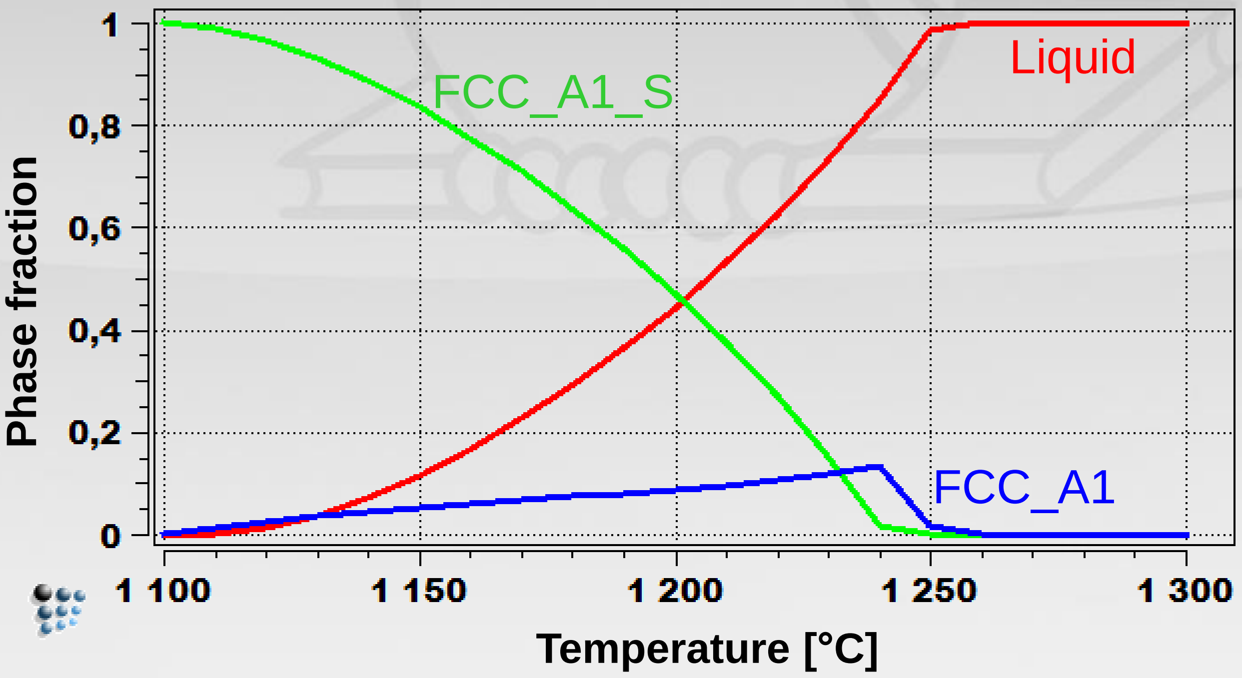
- Microsegregation limits obtained:
  - Core composition: Composition of the very first „α“-phase appearing
  - Intergranular composition: Composition of the liquid phase for a system with some defined liquid content

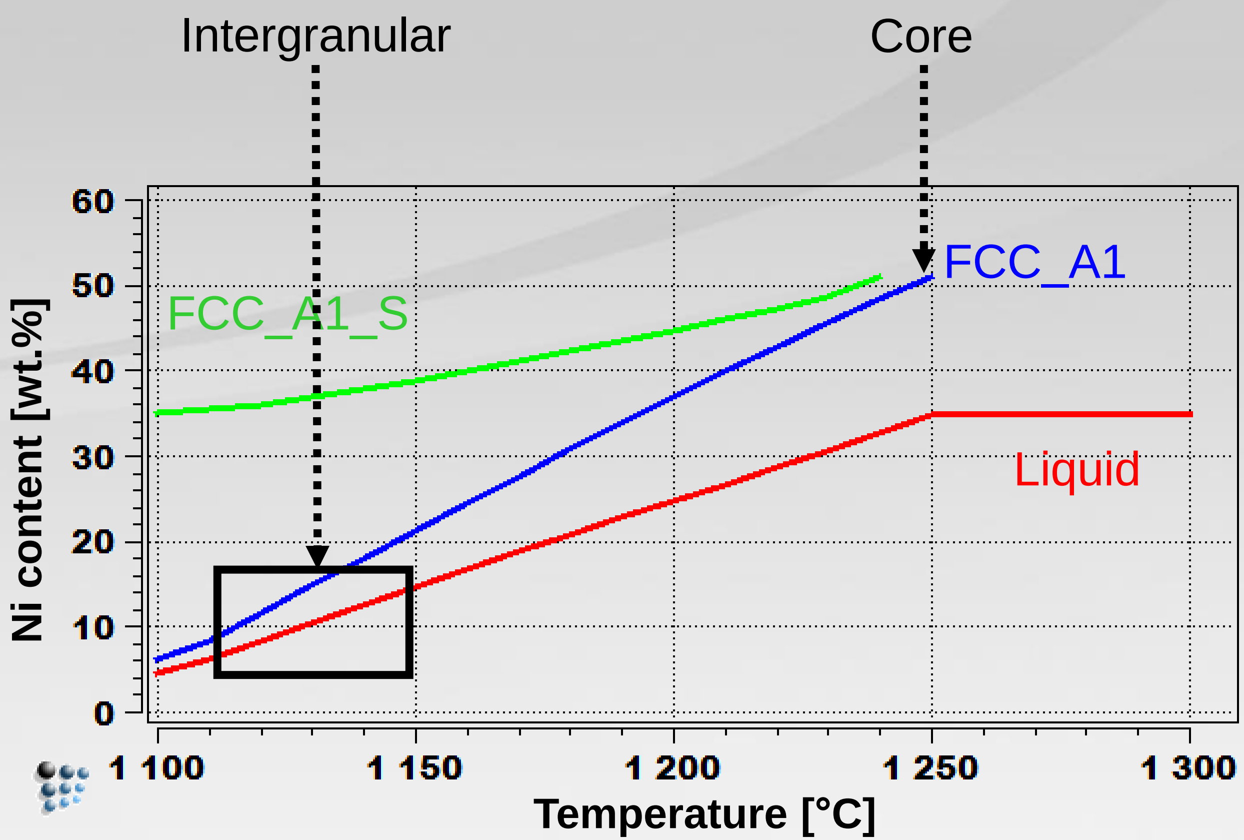
Cooling	Liquid phase fraction [at. %]
Air-cooling	1
Continuous casting	3
Arc furnace	5

MatCalc Engineering

What do I get from it?

- Example: Cu-Ni alloy, 35 wt.% Ni





MatCalc Engineering

What do I get from it?

- Primary precipitate characteristics (if present):
  - Chemical composition
  - Amount (Phase fraction)

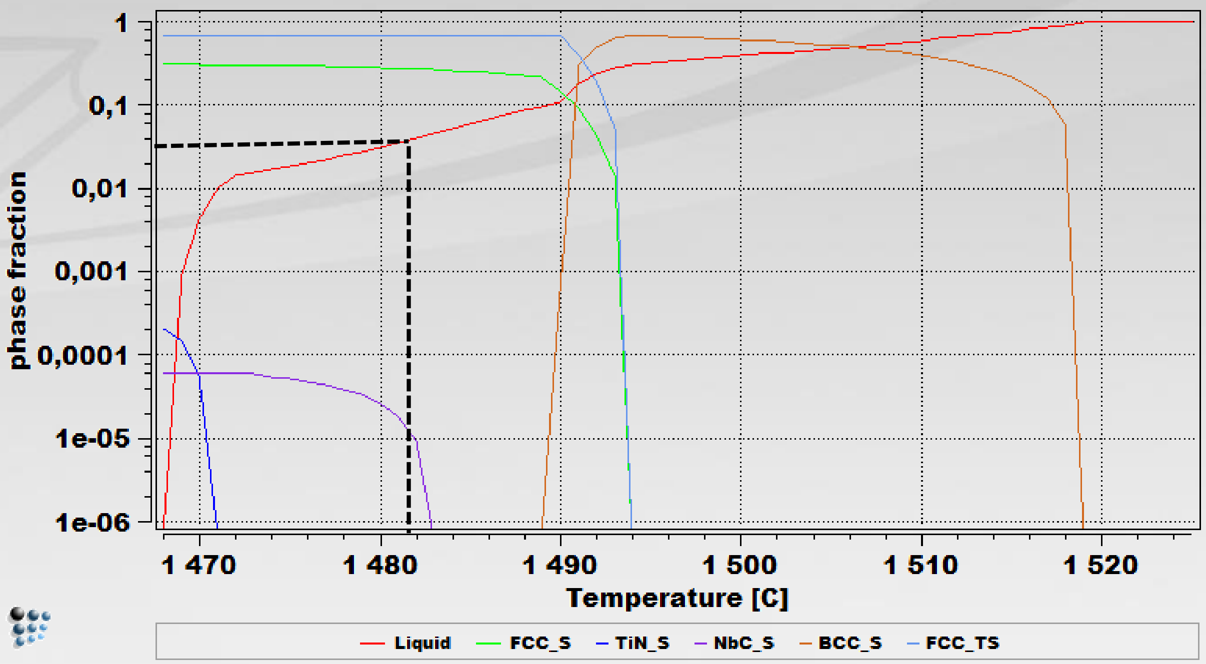
Above parameters are taken from the system with the liquid phase fraction relevant to the solidification cooling rate

Cooling	Liquid phase fraction [at. %]
Air-cooling	1
Continuous casting	3
Arc furnace	5

What do I get from it?

- Example: Fe-Nb-Ti-C-N (Example E20)

- TiN expected as a primary precipitate
- Phase fraction ~1-2*10^{-5}



Application

- Example: Fe-Nb-Ti-C-N (Example E20&P20)

SG-calculation

- Identifying the compositions of solute-enriched and –depleted region
- Identifying the primary precipitates and their amounts

↓

Precipitation kinetics simulation

- Introduction of the precipitate phases representing the primary precipitates
- Simulations performed for both compositions (solute-enriched and –depleted region)

Acknowledgments

- Yao Shan
- Georg Stechauner