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
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
Solid phase composition

- Theoretical estimation: stepped solidification

http://matcalc.tuwien.ac.at/index.php/documentation/detail.php?id=tutorials;t11&media=tutorials;t11;img;t11_figure1v2.png
Solid phase composition

• Theoretical estimation: stepped solidification
Solid phase composition

- Theoretical estimation: Scheil equation

\[ C_S = kC_0 (1 - f_S)^{k-1} \]

- Graph showing the relationship between solid phase composition and temperature.

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

Pro: Nice analytical solution

Contra: Formula dependent on system specification

\[ C_S = kC_0(1 - f_S)^{k-1} \]

Valid for \( k = \text{const.} \) !

\( C_S \)

\( C_0 \)

\( f_S \)
What MatCalc does?

• Stepped solidification $\rightarrow$ SG-calculation
What MatCalc does?

- New equilibrium phase $\alpha$ with solute content $C_{S,1}$ created
- Liquid composition set to $C_{L,1}$
What MatCalc does?

http://matcalc.tuwien.ac.at/index.php/documentation/detail.php?id=tutorials:t11&media=tutorials:t11;img:t11_figure1v2.png
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}
What MatCalc does?

http://matcalc.tuwien.ac.at/index.php/documentation/detail.php?id=tutorials;t11&media=tutorials;t11;img;t11_figure1v2.png
What MatCalc does?

- \( \alpha_S \) formed by merging the previous \( \alpha_S \) and previous \( \alpha \) (adding phase fractions)
- \( \alpha_S \) composition is evaluated from mass balance of the merged phases
- „Dormant“ status set to \( \alpha_S \)
- New equilib. phase \( \alpha \) 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

<table>
<thead>
<tr>
<th>Phase</th>
<th>Fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>FCC_A1</td>
<td>1</td>
</tr>
<tr>
<td>FCC_A1_S</td>
<td>0.8</td>
</tr>
<tr>
<td>Liquid</td>
<td>0</td>
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Equilibrium calculation

SG-calculation

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Example

- Cu-Ni alloy, 35 wt.% Ni
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)
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Primary precipitates
Primary precipitates

• Primary precipitates $\rightarrow$ precipitates formed during the presence of the liquid phase

• Phases coexistent with the liquid phase at the equilibrium calculation $\rightarrow$ strong candidates for the primary precipitates

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

Equilibrium calculation
Primary precipitates

- Primary precipitates are precipitates 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.
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- Phases appearing close to the liquidus should be also checked.

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

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Fe-Nb-Ti-C-N (Example E20)
Modeling of solid-solid transformation
Solid-solid transformation

• A solid phase might transform to another solid phase
• Relevant for the peritectic reaction (e.g. δ-ferrite + liquid $\rightarrow$ 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
    \[ f = 1 - \exp\left(-kT_{frac}^n\right) \quad T_{frac} = \frac{T - T_{stop}}{T_{start} - T_{stop}} \]
  • Koistinen-Marburger
    \[ f = 1 - \exp\left(-nT_{diff}\right) \quad T_{diff} = T_{start} - T \]
• Manual ratio
  • Amounts taken from the table provided by user (Temperature vs. Amount transformed)
Solid-solid transformation

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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 \textbf{before and at} the considered temperature
Solid-solid transformation

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Liquid($C_{L,1}$)

L0 $\rightarrow$ L1 + BCC_A2
Solid-solid transformation

**Technical note**

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**Diagram:**

- **FCC_A1**
- **Liquid(C_{L,2})**
- **BCC_A2_S**

L1 → L2 + FCC_A1
Solid-solid transformation

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Liquid(C_{L,3})

FCC_A1
FCC_A1_S

FCC_A1_TS
BCC_A2_S

L2 \rightarrow L3 + FCC_A1
BCC_A2_S + L2 \rightarrow FCC_A1_TS
Solid-solid transformation

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

Without peritectic transformation

With peritectic transformation
Applications
What do I get from it?

- Microsegregation limits obtained:
  - Core composition: Composition of the very first \(\alpha\) phase appearing
  - Intergranular composition: Composition of the liquid phase for a system with some defined liquid content

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What do I get from it?

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

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What do I get from it?

- Example: Fe-Nb-Ti-C-N (Example E20)
  
  - TiN expected as a primary precipitate
  - Phase fraction $\sim 1.2 \times 10^{-5}$
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