Thermodynamics and Microstructure:
Recent Examples for Coupling of Thermodynamic and Mobility Data to the Software MICRESS®
Outline

- Microstructure Simulation using the Software MICRESS®
- Coupling to Thermodynamic Databases
- Applications:
  - Magnesium Alloys: Grain Size Prediction in AZ31
  - Steels: Hot-Cracking in Continuous Casting
Microstructure Simulation using the Software MICRESS®
The Software MICRESS®

MICRESS: MICRoostructure Evolution Simulation Software

Can be applied to composition, temperature or curvature controlled transformations on the microscale:

- Solidification (dendritic, cellular, peritectic, eutectic)
- Solid state reactions (grain growth, recrystallisation, phase transformations)
- Direct coupling to thermodynamic databases (contains TQ-interface*) or linear phase diagram approximation

*from Thermo-Calc Software, Sweden
1995: first microstructure simulations at ACCESS
1996: multi-phase-field model published
1999: simulations comprising thermodynamic databases
2003: MICRESS is commercially available
2004: MICRESS becomes registered trademark
2005: MICRESS website is online
2006: stress solver incorporated
2007: coupling to external temperature fields
2008: …
MICRESS® uses the phase-field method
Main characteristic: Diffuse Interface, expressed by the phase-field parameter $\phi$

$\phi = f(x,t)$ can be interpreted as a density function for the phase state
Multi Phase-Field Equation used in MICRESS®

rate of change of each phase-field

\[
\dot{\phi}_i = \sum_{j}^{n} \mu_{ij}^* \left[ \sigma_{ij}^* \left( \phi_i \nabla^2 \phi_j - \phi_j \nabla^2 \phi_i + \frac{\pi^2}{2 \eta_{ij}^2} (\phi_i - \phi_j) \right) + \frac{\pi}{\eta_{ij}} \sqrt{\phi_i \phi_j \Delta G_{ij}} \right]
\]

by superposition of pair-wise interactions with neighboring phases

\[ \eta_{ij} = \text{interface thickness} \quad \Delta G_{ij} = \text{driving force} \]
\[ \mu_{ij} = \text{interface mobility (anisotropic)} \]
\[ \sigma_{ij} = \text{interface energy (anisotropic)} \]

diffusion equation

\[
\frac{dc^k(x,t)}{dt} = \nabla \left( \sum_{i=1}^{N} \phi_i D_i^k \nabla c_i^k \right)
\]
Basic Structure of MICRESS®

- Nucleation Models
- Multi-Phase-Field Solver
- Multicomponent Diffusion Solver
- Temperature Solver

Evolution of Phase Distribution
Composition
Temperature

www.micress.de
Thermodynamic Coupling

Calphad Database

ThermoCalc

nucleation undercooling

driving force

solute partitioning

diffusion matrix

latent heat data

loop over time

Nucleation Model

\[ \Delta T_{und} > \Delta T_{crit} ? \]

Multi-Phase-Field Solver

\[ \dot{\phi}_\alpha = \sum_\beta \mu_{\alpha\beta} (\sigma_{\alpha\beta} K + w \Delta G_{\alpha\beta}) \]

Multicomponent Diffusion Solver

\[ \dot{\bar{c}} = \nabla \sum_\alpha \phi_\alpha \bar{D}_\alpha \nabla \bar{c}_\alpha \]

Temperature Solver

ThermoCalc

TQ-Interface

MICRESS®
Application:

Grain Size Prediction in AZ31
Simulation of Microstructure of Mg-Cast Alloys

**Input:** alloy composition, heat extraction rate, distribution of nucleant particles

**Output:** temperature-time curve, grain size, grain morphology, microsegregation, secondary phases …
Thermodynamic Data of Magnesium Alloys

Calphad database of the system Mg-Al-Zn-Ca-Mn

Mg-Al3-Zn1-Mn0.4-Ca

Starting composition for present simulations:

AZ31:
Mg - 3% Al - 1% Zn

Variation of Al, Zn, Ca, Mn
Distribution of Nucleant Particles

Particle density $n$

$$n(r) = \frac{N}{2r} \exp\left[\frac{r}{\bar{r}}\right]$$

Nucleant particles: grain refiner particles, impurities
Integrated Nucleation Model

Nucleation-Model

\[ \Delta T_{\text{crit}}(r) < \Delta T(\bar{c},T) \] ?

Multi-Phase-Field-Solver

Multicomponent Diffusion-Solver

Temperature-Solver

nucleant positioning

nucleant distribution

new nucleus

critical undercooling

nucleants with different radii

density

radius

\[ \Delta T_{\text{crit}}(r) = \frac{2\sigma}{\Delta S \cdot r} \]
Simulations with Variation of Aluminium Content

Mg-3%Al-1%Zn  Mg-6%Al-1%Zn  Mg-9%Al-1%Zn

AZ31  increased aluminium content  decreased grain size  AZ91
Principal Effect of Solute on Grain Refinement

aluminium concentration around a growing grain

higher concentration \(\rightarrow\) higher solute pile-up

\(\rightarrow\) growth restriction

\(\rightarrow\) higher maximal undercooling

higher concentration higher solute pile-up

3% Al

6% Al

9% Al

undercooling \(T_{\text{Liq}}(c_0) - T\) [°C]

first nucleation

\(\Delta T_{\text{min}}\)

\(\Delta T_{\text{max}}\)

3% Al
6% Al
9% Al
Evaluation of Grain Size dependent on Aluminium Concentration

Simulation Parameters
Software: MICRESS
Method: Phase-field
1000 x 1000 cells
\( \Delta x = 2 \, \mu m \)
d\( \frac{dQ}{dt} = -5 \, \text{Js}^{-1} \, \text{cm}^{-3} \)

mean grain radius [\( \mu m \)]

aluminium concentration [wt\%]

Mg-x\%Al-1\%Zn

Al-Variation

Mg-3\%Al-1\%Zn
Evaluation of Grain Size dependant on Solute Concentration

Simulation Parameters
Software: MICRESS
Method: Phase Field
1000 x 1000 cells
$\Delta x = 2 \ \mu m$
d$Q / dt = -5 \text{ Js}^{-1} \text{ cm}^{-3}$

mean grain radius $[\mu m]$
Comparison with Growth Restriction Theory

Grain size is described in linear approximation to the inverse of the Growth Restriction Factor

\[ r_{\text{mean}} = a + \frac{b}{\text{GRF}} \]

的行为 Mn 只能理解为多组元效应！

（应用于 D. St John, M. Easton 对 Mg 合金）
Application:

Hot Cracking in Continuous Casting
Example: Continuous steel casting – initial stage

Problem at initial stage of solidification (first few millimeters):
highly non-stationary and non-linear temperature profile

1D temperature field (low resolution)

“normal” 2D simulation domain (high resolution) is coupled to 1D temperature field

→ simulation with realistic temperature profiles

low-alloyed ferritic steel:

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<th></th>
<th>C</th>
<th>Si</th>
<th>Mn</th>
<th>P</th>
<th>S</th>
<th>Cr</th>
<th>Cu</th>
<th>N</th>
<th>Ni</th>
<th>Nb</th>
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<td>0.047</td>
<td>0.022</td>
<td>0.13</td>
<td>0.011</td>
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<td>0.009</td>
<td>0.004</td>
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</tr>
</tbody>
</table>
Temperature and Fraction Solid Curves

T curves

Mn/wt%

f_s curves

Virtual EDX
Determination of Zero Ductility Temperature (ZDT) using Critical Fraction Solid of 0.95

important for hot cracking!
Microstructure Simulation of Peritectic Alloy B

Alloy B:

- T(95%) = 1438°C
- T(99%) = 1405°C
- T(FCC) = 1432°C
- T(Ti4C2S2) = 1423°C
- T(MnS) = 1406°C
- T(TiN) = 1395°C

| Fe  | C   | Si  | Mn  | P  | S  | Al  | Cr  | Cu  | Mo  | N   | Ti  | Ni  |
|-----|-----|-----|-----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|
| Bal.| 0,225 | 0,078 | 1,66 | 0,012 | 0,0015 | 1,526 | 0,021 | 0,019 | 0,005 | 0,002 | 0,003 | 0,021 |
Microstructure Simulation of Peritectic Alloy B: Rappaz-Kriterium

\[ \dot{\varepsilon}_{krit} = \sum_i \frac{G}{(1 + \beta_i)B_i} \left[ \frac{\lambda_2^2 G \Delta p_{max}}{180 \mu} - v \sum_i \beta_i A_i \right] \]
Segregation Band Alloy B

increased hot cracking potential!
Thank you for your attention!