Thermodynamic, kinetic and phase transformation calculations in the field of single crystal nickel based superalloys

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ThermoCalc User Meeting - Aachen
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Agenda

- Nickel-based alloys as a key for energy production
- Thermodynamic and kinetic databases for alloy development
- Heat treatment modelling
- Simulation of microstructure evolution
- Summary
Combined cycle power plant

Efficiency (2007): ca. 58% (330 g CO₂ / kWh)
Aim 2020: ca. 63% (300 g CO₂ / kWh)

1st stage blade
250 mm, 4.3 kg
1 MW
50 Hz
10 t
1000 °C
3 yrs
10,000,- $
Efficiency of fossil power plants

Development of efficiency

Relation of efficiency and process temperature

turbine outlet temperature is 500 °C

data according to Siemens AG and DPG (2005)

⇒ efficiency increase is always related to higher material temperatures
Development of nickel-based superalloys

- Single crystalline
- Directionally solidified
- Polycrystalline
- Wrought alloys

Temperature capability of nickel-based superalloys

Year of development

Service temperature

Harada et al. (2003) IGTC2003
Turbine blades

1st stage, SGT5-4000F, Siemens AG

polycrystalline, directionally solidified, single crystalline
Turbine blades

1\textsuperscript{st} stage, SGT5-4000F, Siemens AG

- polycrystalline
- directionally solidified
- single crystalline
Single crystal nickel-based superalloys

γ + γ'-microstructure gives unique creep properties

typical alloying elements (ca. 8 – 10):
Ni-Al-Co-Cr-Mo-Re-Ru-Ta-Ti-W-B-Zr-Y
Material / process simulation at Institute WTM

thermodynamics
  *ThermoCalc*

process simulation (temperature-, fluid flow)
  - *Flow3D*
  - *ProCAST*
  - *inhouse Lattice Boltzmann code*

diffusion
  *DICTRA*

phase transformations
  *TC-PRISMA*

microstructure
  *MICRESS*

mechanics (finite elements)
  *ABAQUS*

computer-aided alloy development
  *inhouse software (MultOPT)*

Institute WTM / NMF
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Fields of application

- **Prediction of:***
  - Liquidus (melting) temperature
  - \(\gamma'\)-phase fraction
  - \(\gamma'\)-solvus temperature
  - TCP-phase solvus temperatures

- **Limitations:***
  - "Exotic" alloying elements are not available
  - Most commercial databases are not changable and the exact parameters are often not accessible
  - Calculations for untypical compositions may be critical
  - Calculations are only valid for stable equilibrium
Verification of commercial database TTNi7

Phase compositions calculated with TTNi7

Diffusion database development for Ni-Ge


![Graph showing diffusion coefficients for Ni-Ge alloys at different temperatures.](graph.png)

**Interdiffusion**

- NiGe8
- NiGe1
- PWA1483
- René N5

**Diffusion Coefficient** $D / \text{m}^2\text{s}^{-1}$

**1/T / 1/K**

- $6.5 \times 10^{-4}$
- $6.7 \times 10^{-4}$
- $7.0 \times 10^{-4}$
- $7.2 \times 10^{-4}$

**Ge Impurity**

- $1250 ^\circ\text{C}$
- $1200 ^\circ\text{C}$
- $1150 ^\circ\text{C}$

**Self Diffusion**

- Rettig et al. (2011)
- Hirano et al. (1962)
- Mantl et al. (1983)

**DICTRA-database from diffusion couple measurements**
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A multicomponent, multiphase precipitation model

**Idea of model**

- Loop for all timesteps
  - Loop for all precipitate types
    - New nucleation
    - Growth of all existing particles
    - Total removal of solute from matrix
  - Driving force from CALPHAD
    - Nucleation rate
    - Loop for all particles
      - Growth rate using CALPHAD
        - Volume change
        - Solute removal from matrix

red: new multicomponent model
A multicomponent, multiphase precipitation model

Idea of model

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Modelling of TCP-phase precipitation

multicomponent Kampmann-Wagner-model (coupled to ThermoCalc and DICTRA)

databases: TTNi8 + MobNi1

FIB-tomography

9 x 7 x 6 μm³

experimental 3rd generation alloy
ASTRA1-20

K. Matuszewski, R. Rettig et al.

experimental data: Sato et al. (2006) Scripta Mat

9 x 7 x 6 μm³
Modelling of TCP-phase precipitation
Driving force influences precipitate length

the large difference in the driving force in both alloys is the reason for the very different precipitate lengths

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- Fields of application of thermodynamic and kinetic simulations
- Advanced modelling using CALPHAD-calculations as a basis
  - Heat treatment simulation
  - Precipitation simulation