Numerical optimization of solution heat treatments of single crystal nickel-based superalloys: Methods and validation

R. Rettig, F. Müller, R.F. Singer
Materials Science, University of Erlangen, Germany

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Agenda

- Nickel-based superalloys: metallic high temperature materials
- Solution heat treatment of superalloys
- Validation of thermodynamic and kinetic databases
- Fast calculation of property maps of microstructures
- Summary
Combined cycle power plant

- efficiency (2011): ca. 60% (330 g CO₂ / kWh)
- aim 2020: ca. 63% (300 g CO₂ / kWh)

Siemens AG

Keppel, Alstom, Cooretec Workshop, 2006
Efficiency of fossil power plants

Development of efficiency

data according to Siemens AG and DPG (2005)

Relation of efficiency and process temperature

turbine outlet temperature is 500 °C

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

Harada et al. (2003) IGTC2003

- Temperature capability of nickel-based superalloys (breaking after 1000 h at 137 MPa)

- Year of development vs. max. service temperature (°C)

- Single crystals
- Directionally solidified
- Conventionally cast (globulitic)
- Forged

- TMS-162
- CMSX-4
- MarM247
- IN792
- Waspalloy

**Turbine blades**

1st stage, SGT5-4000F, Siemens AG

- Polycrystalline
- Directionally solidified
- Single crystalline

5 cm

2 cm
Turbine blades

1st stage, SGT5-4000F, Siemens AG

polycrystalline
directionally solidified
single crystalline
Agenda

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Heat treatment cycle for superalloys

Aims:
- reduction of dendritic segregation

Heat treatment cycle:
- solution heat treatment: 1340 °C, 16 h

Dendritic segregation (ASTRA1-20):
- standard heat treatment (CMSX-4)

Typical values for Re-containing alloys:
Heat treatment cycle for superalloys

Aims:
- reduction of dendritic segregation
- dissolution of eutectic phases

Heat treatment cycle:
- Solution heat treatment at 1340 °C for 16 hours

Typical values for Re-containing alloys:
- Eutectic phases
- Typical directionally solidified microstructure
Heat treatment cycle for superalloys

**Aims:**
- reduction of dendritic segregation
- dissolution of eutectic phases
- **precipitation of well-defined cubic \( \gamma' \)-phase particles**

Typical values for Re-containing alloys:

- Solution heat treatment:
  - \( T = 1340 \, ^\circ \text{C}, \, 16 \, \text{h} \)
  - \( T = 1140 \, ^\circ \text{C}, \, 2 \, \text{h} \)
  - \( T = 870 \, ^\circ \text{C}, \, 24 \, \text{h} \)

- \( \gamma' \)-precipitation aging:
  - \( T = 1140 \, ^\circ \text{C}, \, 2 \, \text{h} \)

**Microstructure:**
- Typical coherent \( \gamma/\gamma' \)-microstructure
- \( \gamma' \)-phase particles
- \( \gamma \)-matrix

5 \( \mu \text{m} \)
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Verification of commercial database TTNi7

\( \gamma \) and \( \gamma' \)-phase composition calculated with TTNi7

Rettig et al.
Defect Diffus.
Forum (2009)

good agreement

bad agreement
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Thermodynamic properties of the microstructure

CMSX-4

measured as-cast microsegregation

calculated solidus temperature distribution => incipient melting prediction

Rettig et al., Model. Sim. Mat. Sci. Eng.(2014)
Efficient calculation of microstructure maps

Difficulty:

- The calculation of a typical 250 x 250 pixel map takes around 1h
- Application in evaluation of heat treatment simulations requires calculation times smaller than 5 minutes

Solution:

- Application of surrogate models ("nonlinear interpolation")

Algorithm:

Rettig, Singer, Modelling and Simulation in Materials Science and Engineering (2014)
Surrogate modelling

Aim:
- Replacement of a computationally expensive CALPHAD-property function by a cheaper one („model of the model“)

Important methods:
- Response Surface Models („polynomial fitting“)
- Artificial Neural Networks
- Inverse Distance Weighting
- Kriging method

an open-source library is available for MATLAB (DACE-library, University of Denmark)

„non-linear fitting“ of the CALPHAD-property functions based on a small number of nodes

$\gamma'$-content at 1100 °C (CMSX-4)
Classification of the microstructure

Classification by magnitude of the compositional distance vector relative to a reference point

Rettig et al., MSMSE(2014)
Classification of the microstructure

Classification by magnitude of the compositional distance vector relative to a reference point

Rettig et al., MSMSE(2014)
Classification of the microstructure

Classification by magnitude of the compositional distance vector relative to a reference point

Rettig et al., MSMSE(2014)
Classification of the microstructure

Classification by magnitude of the compositional distance vector relative to a reference point

80 random nodes per class
Algorithm parameters

Optimum parameters:
- 80 nodes per class
- 15 classes

Achieved speed-up:
- around 30 for a single calculation
- around 300 for repeated calculations

Rettig et al., MSMSE(2014)
Application: $\gamma'$-solvus temperature distribution in CMSX-4

Quality of the interpolation:

- interpolation error is below 1 °C for most areas
- slightly larger errors in the interdendritic regions

Rettig et al., Model. Sim. Mat. Sci. Eng.(2014)
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Summary

- Development of a high-performance algorithm for the calculation of microstructure mappings

- New possibility for the post-processing of phase-field simulations predicting the homogenization during solution heat treatments

- The Kriging-method has a high general potential for improving speed when applying the CALPHAD-method