Computational Steel Design – Chances and Limits of Materials Modelling

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• Introduction ICMPE: Integrative Computational Materials and Process Engineering
• AixViPMaP – a platform concept for ICMPE
• Example 1: Al-reduced case hardening steel for high temperature carburising processes
• Example 2: Ab initio based design of HMS: High Manganese Steels
• Summary and Outlook
Numerical simulation support for cold rolled steel development

- High level of innovation
  - Risk of implementation
  - Costs of implementation
  - Time of implementation

- Low level of knowledge

<table>
<thead>
<tr>
<th>Steel development</th>
<th>HMnS</th>
<th>AHSS</th>
<th>HSLA</th>
</tr>
</thead>
<tbody>
<tr>
<td>Start Modelling</td>
<td>2000</td>
<td>1990</td>
<td>1980</td>
</tr>
<tr>
<td>Start indust. application</td>
<td>2010</td>
<td>1990</td>
<td>1970</td>
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- Model approaches
  - ab initio
  - CP
  - RVE
  - DDE
  - CDM
  - CalPhad
  - TC
  - PFM
• Sound understanding of different materials phenomena, process parameters and process facilities entities
• Integrated, harmonised virtual modelling methodologies and tools
• Integration of input/output between virtual and real world
• Inverse assessment of product creation chains
• Integration of logistic and factory planning aspects
• “First time right” approaches
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All results in the same format – one viewer for all scales

- e.g. paraview (freeware from www.kitware.org)

... and microscale ...

... can be presented in one frame
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Simulation concept of process chain for gear components
• Eco-friendly and high efficient **case hardening** request for high temperature carburizing treatments.

• **Grain size control** is needed for fatigue properties.

• Grain growth can be prevented by **microalloying**, but complex process conditions need to be considered.

• Prediction of particle fraction and size + grain size development and distribution is simulated by **ICMPE**.
Material: 25CrMo4 + Nb/Ti

<table>
<thead>
<tr>
<th></th>
<th>C</th>
<th>Si</th>
<th>Mn</th>
<th>Cr</th>
<th>Mo</th>
<th>Ni</th>
<th>V</th>
<th>Al</th>
<th>N</th>
<th>Ti</th>
<th>Nb</th>
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<tbody>
<tr>
<td></td>
<td>0.24</td>
<td>0.22</td>
<td>0.89</td>
<td>0.92</td>
<td>0.43</td>
<td>0.18</td>
<td>0.008</td>
<td>0.023</td>
<td>0.016</td>
<td>0.009</td>
<td>0.034</td>
</tr>
</tbody>
</table>

Microalloyed Gear Steels
Experimental Procedure
Experimental observations: complex distribution of different precipitates

- Particles with different sizes and shape factors: AlN, NbC and Ti(C,N)
- Interaction of different particles
- Many different process routes and process parameters
Simulation results during process chain

- Empirical modelling is successfully applied for particle size development in different process steps.
- Thermodynamic databases provide input parameter.
- Additional experimental input is helpful for exact quantification.
• Precipitation evolution and calculation of Zener force through the whole process.
• Simulation of grain growth by using Zener force as a function of precipitation state.
Application of ICMPE for process parameter variation

- Increasing of heating rate along the whole process chain, variation of austenitization temperature.

- Recrystallization annealing versus direct case hardening after cold forming.

- Increasing of case hardening temperature and change of initial precipitation state.
Case hardening 1050 °C – 1h30 (after analysis of austenite grain size)

Results of process chain variation

Increase of pinning force due to increase of heating rate

Small improvement of pinning force via small variation of austenitization temperature or shorten of process chain

Decrease of pinning force by increase of austenitization temp. up to 1200 – 1300 °C
• Al reduction is asked for **cleanliness improvement**.
• For reaching the same precipitation level at 1050 °C as a reference Nb alloyed 25CrMo4 steel, Al reduction has to be answered by an increase of **Nb content**.
• Additionally, for Nb-(C,N) an increase in **solution temperature** is needed.
• Conclusion: a combined development of alloy and process parameters is needed in order to realize this new steel concept.

**Design of an Al-reduced case hardening steel**
Process chain:
- Continuous Casting,
- Forging,
- FP Annealing,
- Case Hardening 1100 °C

Assumption:
No Segregation Effects
Evolution of particle fraction

- Hot Forging
- Case Hardening
- Al-free
  - 700 ppm Nb
  - 30 ppm Al

Reference
Evolution of particle size

Reference

Al-free

700 ppm Nb
30 ppm Al

Mean particle size, nm

Time, h

Mean particle size, nm

Time, h
Evolution of Zener force

Reference

Al-free
700 ppm Nb
30 ppm Al

Evolution of Zener force
Grain size distribution after case hardening treatment

Customer specification

Grain size distribution after case hardening treatment
Integrative Computational Materials and Process Engineering is a promising approach for efficient process and materials design.

The integrative simulation of process chains needs the definition of an integrative platform covering scales, materials and process steps for the communication between different approaches and simulation programs.

As a demonstrator, the process chain for gears has been investigated in a parameter study. Furthermore, a new Al reduced steel has been designed that shows grain size stability for high temperature carburising.

The further extension of the platform towards production planning will be a main future development direction.
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Different deformation mechanisms control plasticity

Mechanical properties of new steel concepts on Mn basis

![Graph showing the relationship between Mn content and tensile strength/uniform elongation for different steel concepts: AHSS, Medium Mn TRIP, High Mn TRIP, TWIP, MBIP, and MBIP + Al.](image)

- **Materials SFB 761**
- **AHSS**: Advanced High Strength Steels
- **Medium Mn TRIP**: Martensite Ferrite Bainite Transformation Induced Plasticity
- **High Mn TRIP**: High Manganese Transformation Induced Plasticity
- **TWIP**: Twinning Induced Plasticity
- **MBIP**: MicroBand Induced Plasticity
- **MBIP + Al**: MicroBand Induced Plasticity with Aluminum

VII, IV, II, I, III, MBIP:

MBIP: MicroBand Induced Plasticity
Structure determination by *ab initio*-calculations

Where is C located in fcc-Fe-Mn? → Supercell models

Energy comparison of all configurations → Mn-rich octahedron preferred

Energy difference relative to most stable configuration of C in Fe-Mn-C-Supercell
Why is C located there?

Assumption: stronger Mn-C bond

Not relevant

ICOHP Data:
C-Mn: -4.31 eV
C-Fe: -4.43 eV

C-Fe bond 0.12 eV stronger

ICOHP: Integrated Crystalorbital-Hamilton-Population

Bonding interaction of C with Fe and Mn in Fe-Mn-C supercell
Comprehension with \textit{ab initio}-calculations

Why is C located there?

\rightarrow Bonding analysis

Volume expansion due to C causes

\checkmark Fe-Fe-distance from 101\% to 106\%

\checkmark Mn-Mn-distance from 93\% to 99\% (corresponding to ideal values)

\checkmark Fe-Fe-bond weaker than Mn-Mn-bond due to C

assumption: stronger Mn-C-bond

\checkmark not relevant

investigation of Mn-Mn and Fe-Fe bond

\checkmark relevant

Bonding interaction of Mn-Mn and Fe-Fe in Fe-Mn-C supercell
Different deformation mechanisms in high manganese steels

Dislocation interaction

homogenous dislocation movement

inhomogenous dislocation movement

Lattice interaction

TRIP - effect

TWIP - effect
The **Stacking Fault Energy (SFE)** defines the active modes of plasticity: dislocation glide, TRIP, TWIP, etc.

![Diagram showing the relationship between Temperature, Manganese content, and deformation mechanisms (TRIP, TWIP)]
\[ \gamma_{fcc} = 2 \rho \Delta G^{\gamma \rightarrow \varepsilon} + 2\sigma^{\gamma / \varepsilon} \]

Different types of Mechanism Maps

TWIP

TRIP

Temperature [K]

Carbon content [wt.%]

Manganese content [wt.%]

300 K

0.6 wt.% C

[mJ/m²]

[mJ/m²]
Temperature controls deformation mechanism of TWIP 900

Temperature:
- 173K
- 273K
- 373K

SFE \([\text{mJ/m}^2]\):
- 0.017
- 0.026
- 0.042

Graph showing the relationship between true stress and true strain for different temperatures (173K, 273K, 373K) of TWIP 900.
Temperature influence on flow behaviour

\[ \sigma = f(\dot{\varepsilon}, T, \rho_c, \rho_w, V_{Twin}) \]

- \( \sigma \): stress
- \( \varepsilon \): strain rate
- \( T \): temperature
- \( \rho_c \): dislocation density in cell center
- \( \rho_w \): dislocation density at cell boundary
- \( V_{Twin} \): Volume fraction of twins

Stress strain curves; Comparison experiment & model
Influence on strain hardening behaviour

\[ \sigma = f(\dot{\varepsilon}, T, \rho_c, \rho_w, V_{\text{Twin}}) \]

\( \sigma \): stress, \( \dot{\varepsilon} \): strain rate, \( T \): temperature, \( \rho_c \): dislocation density in cell center, \( \rho_w \): dislocation density at cell boundary, \( V_{\text{Twin}} \): Volume fraction of twins
SFE controls plastic deformation mechanisms

High Mn steel

SFE

SLIP

Kocks - Mecking

Austenite

Kocks - Mecking

TWIP

Mixture Law

Austenite

Kocks - Mecking

Stress Ind. Twinning

Kocks - Mecking + Bouaziz

TRIP

Mixture Law

Austenite

Kocks - Mecking

Strain Ind. Martensite

Kocks - Mecking + Olsen Cohen

Algorithm for a mechanism based flow law
RVE calculation of numerical tensile test
In situ bending test of pre-strained tensile specimens

- *in situ* bending device
- max. force 5000 N
- max. displacement 15 mm
- Temperature up to 800 °C
In situ bending test of pre-strained tensile specimens

- Pre-strained tensile specimen (95% of TEL)
- 22Mn0.6C hot rolled (grain size 2 μm)
In situ bending test of pre-strained tensile specimens

- Twins and twin intersections are visible
- Surface roughening
- Fracture occurs on surface at shear bands
Cohesive zone model for 22Mn0.6C (233 K)

RVE simulation using damage model

Experiment

continuum elements

failed cohesive elements
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Chances:
- Development of robust processes/materials by sensitivity analysis
- Quantitative comprehension of process – material interaction
- Full exploitation of material properties
- Improved and accelerated knowledge driven design of tailored materials and processes

Limits:
- Process inherent irregulations
  - Segregation, distortion, inclusions (rare events)
- Competition of phenomena
  - Failure mechanisms
  - Deformation mechanisms
- Quantitative accuracy of ab initio methods
- Computational limits
The examples in this talk have been taken from

- Industry financed research projects

S. Konovalov, RWTH Aachen University

- Collaborative Research Center SFB ab inito

Dr. von Appen, Prof. R. Dronskowski, Dr. A. Saaed-Akbari, R. Twardowski, RWTH Aachen University

Dr. F. Roters, D. Steinhoff, MPI Düsseldorf

The financial support of Deutsche Forschungsgemeinschaft is gratefully acknowledged.