SFB 761 „Stahl ab initio“

Quantum mechanics guided design of new Fe based materials
Steel \textit{ab initio}

1. Motivation / Background
   • Material-Development
   • Method-Development

2. General Information
   • Structure / Participants (PB-, TP-Leiter)

3. Scientific progress / first results
   • Modelling
   • Material processing
   • Evaluation

4. Integrated Graduate School

5. Future plans / Vision

---

Agenda
1. Motivation / Background
   • Material-Development
   • Method-Development

2. General Information
   • Structure / Participants (PB-, TP-Leiter)

3. Scientific progress / first results
   • Modelling
   • Material processing
   • Evaluation

4. Integrated Graduate School

5. Future plans / Vision
### Chemical Composition of Sheet Steels

#### Trend to higher alloying contents

<table>
<thead>
<tr>
<th>Steel Group</th>
<th>Fe in wt.%</th>
<th>Alloying elements in wt.%</th>
<th>Tramp elements in wt.%</th>
</tr>
</thead>
<tbody>
<tr>
<td>DDQ</td>
<td>98</td>
<td>Al, Nb, Ti (ca. 1)</td>
<td>&lt; 1</td>
</tr>
<tr>
<td>Stainless</td>
<td>73</td>
<td>Cr, Ni (ca. 26)</td>
<td>&lt; 2</td>
</tr>
<tr>
<td>HSLA</td>
<td>98</td>
<td>Nb, Ti, V (ca. 1)</td>
<td>&lt; 1</td>
</tr>
<tr>
<td>AHSS</td>
<td>96</td>
<td>Mn, Si, Al, Nb, Ti, Cr (ca. 3)</td>
<td>&lt; 1</td>
</tr>
<tr>
<td>Fe-Mn Steels</td>
<td>72</td>
<td>Mn (ca. 25)</td>
<td>&lt; 3</td>
</tr>
</tbody>
</table>
## Trend to knowledge based development

<table>
<thead>
<tr>
<th>Steel group</th>
<th>Year</th>
<th>Development Principle</th>
<th>Motivation</th>
</tr>
</thead>
<tbody>
<tr>
<td>stainless steels</td>
<td>1910</td>
<td>empirical V2A</td>
<td>chemical industry</td>
</tr>
<tr>
<td>microalloyed steels</td>
<td>1960</td>
<td>process driven, TM-rolling, TEM</td>
<td>crude oil / natural gas industry</td>
</tr>
<tr>
<td>multiphase steels</td>
<td>1990</td>
<td>phenomenological, microstructure design, analytic models</td>
<td>automotive industry</td>
</tr>
<tr>
<td>Fe-Mn-C-alloys</td>
<td>2000</td>
<td>ab initio Scale Hopping knowledge driven</td>
<td>light weight construction, safety, energy efficiency</td>
</tr>
</tbody>
</table>

**Motivation for steel development**
Trend to complex microstructures

<table>
<thead>
<tr>
<th>Steel group</th>
<th>Parameters</th>
<th>Deformation mechanisms</th>
</tr>
</thead>
<tbody>
<tr>
<td>Microalloyed steels</td>
<td>• Grain size&lt;br&gt;• Grain shape&lt;br&gt;• precipitates</td>
<td>• homogeneous dislocation glide</td>
</tr>
<tr>
<td>Multiphase steels</td>
<td>+&lt;br&gt;• local chemical composition</td>
<td>+</td>
</tr>
<tr>
<td>Fe-Mn-C steels</td>
<td>• Stacking fault energy&lt;br&gt;• Thermodynamics&lt;br&gt;• Phase stability</td>
<td>• inhomogeneous dislocation glide</td>
</tr>
<tr>
<td></td>
<td>+</td>
<td>+</td>
</tr>
<tr>
<td></td>
<td>• TRIP - Effect&lt;br&gt;• TWIP- Effect</td>
<td></td>
</tr>
</tbody>
</table>
Characteristics of Fe-Mn-C-alloys

• Next to conventional bcc-Fe-C-steels and fcc-Fe-Cr-Ni-steels, the system Fe-Mn-C displays a high potential for the development of a new matrix of Fe based alloys.

• Fe-Mn-C-alloys are particularly well suited for the planned new systematic approaches of material- and method-development.

• All known strain hardening mechanisms do occur in one alloy system.

• Due to the strong dependency of the stacking-fault-energy (SFE) this alloy system is especially suitable for thermodynamic modelling.

Reasons for Fe-Mn-C alloy-selection
Steell *ab initio*

1. Motivation /Background
   - Material-Development
   - Method-Development

2. General Information
   - Structure / Participants (PB-, TP-Leiter)

3. Scientific progress / first results
   - Modelling
   - Material processing
   - Evaluation

4. Integrated Graduate School

5. Future plans / Vision

---

RWTH
Modelling on different scales are used selectively

“Scale-Hopping” approach:
⇒ Efficient design of new steels and processes through focus on core mechanisms

Atomic Scale:
e.g. calculation of the stacking fault energy

Macroscopic Scale:
e.g. calculation of the local strains

“Scale-Hopping” approach:
⇒ Efficient design of new steels and processes through focus on core mechanisms

Microscopic Scale:
e.g. calculation of interphase kinetics

Mesoscopic Scale:
e.g. calculation of the strain hardening as a function of different strengthening mechanisms

Atomic Scale:
e.g. calculation of the stacking fault energy

Modelling Techniques
Quantum mechanically driven material design

Schrödinger-equation: \[ H\Psi = E\Psi \]

for many-particle system consisting of electrons and nuclei

- Many-body wave function
- Total energy
- Hamiltonian incl. interaction potentials

Atoms
Ab initio calculations of solids are efficiently performed within density functional theory.

Schrödinger-equation: \( H\Psi = E\Psi \) for many-particle system consisting of electrons and nuclei.

- Many-body wave function
- Total energy
- Hamiltonian incl. interaction potentials

Motivation for method development

Density functional theory
- Universal approach
- No empirical assumptions
- No fitting to experiment
*ab initio* approaches treat technical relevant alloy systems

Parameterfree determination of:

- Electron structure / chemical bonds
- Atom configuration / crystal structures
- Elastic / mechanical properties
- Energy and dynamics of defects
- Magnetic order

Motivation for method development
Steel *ab initio*

- Development of new methods for material- and process-development based on *ab initio* approaches.
- Material-design of a new class of structural materials.
- Speed-up of development-time and reduction of efforts for material development using „Scale-Hopping".
Precise and experimental results expected

- Laboratory production and characterization of materials with Fe-Mn-C-matrix.
- Usage of ab initio methods in order to predict phase transformations and changes in mechanisms.
- Quantification of the influence of chemical composition, temperature and other parameters on strain hardening mechanisms.
- Extensive characterization of new material group for different fields of application.
- Recommendation of production parameters for existing or new processing routes.
- Enhancement and validation of ab initio methods für model systems and real materials.

Results after 4 and 8-12 years
Steel *ab initio*

1. Motivation /Background / General Information
   - Material-Development
   - Method-Development

2. General Information
   - Structure / Participants (PB-, TP-Leiter)

3. Scientific progress / first results
   - Modelling
   - Material processing
   - Evaluation

4. Integrated Graduate School

5. Future plans / Vision
Close Connection between the RWTH and the MPIE for the SFB leadership

**Speaker**

Prof. W. Bleck (RWTH, IEHK)

**Deputy Speaker**

Prof. D. Raabe (MPIE)

**Department Speakers**

**A: THEORY**

Prof. Dronskowski (RWTH, IAC)

**B: PROCESSES**

Prof. Hirt (RWTH, IBF)

**C: EVALUATION**

Prof. Mayer (GfE)

Organisation of the SFB
RWTH: 13 Partprojects – MPIE: 4 Partprojects

A1 Dronskowsk

ab initio Quantum Chemistry

A2 Neugebauer/Hickel

ab initio Thermodynamic

A3 Schneider / Hallstedt

Thermodynamic

A4 Emmerich

Phasefield-Simulation

A5 Bleck

Mechanism-Maps

A6 Gottstein / Mohles

Interfaces

A7 Roters

Crystalplasticity

B1 Senk

Solidification

B2 Hirt

Forming

B4 Molodov / Gottstein

Annealing

C1 Mayer

Microstructure-Analysis

C2 Bleck

Strengthening Mechanisms

C3 Schneider / Music

Local Mechanical Properties.

C4 Raabe / Zaefferer

Texture & Anisotropy

C5 Winning

Defects & Stresses

C6 Prahl

Damage & Failure

RWTH: 13 Partprojects

MPIE: 4 Partprojects

SFB-constitution
RWTH: 13 Partprojects – MPIE: 4 Partprojects

A1 Dronskowski 
ab initio Quantum Chemistry

A2 Neugebauer/Hickel 
ab initio Thermodynamic

A3 Schneider / Hallstedt 
Thermodynamic

A4 Emmerich 
Phasefield-Simulation

A5 Bleck 
Mechanism-Maps

A6 Gottstein / Mohles 
Interfaces

A7 Roters 
Crystalplasticity

B1 Senk 
Solidification

B2 Hirt 
Forming

B4 Molodov / Gottstein 
Annealing

C1 Mayer 
Microstructure-Analysis

C2 Bleck 
Strengthening Mechanisms

C3 Schneider / Music 
Local Mechanical Properties

C4 Raabe / Zaefferer 
Texture & Anisotropy

C5 Winning 
Defects & Stresses

C6 Prahl 
Damage & Failure

Korea-Participants

[Diagram showing RWTH and MPIE projects with Korea participants and PP not taking part]
Steel *ab initio*

**Participation at International Conferences with special SFB-sessions**

- **MSE-Nürnberg**
  - Materials Science & Engineering
  - September 1st-4th 2008

- **THERMEC Berlin**
  - August 25th-29th 2009

- **MRS-FallMeeting Boston**
  - Nov. 29th- Dec. 3rd 2010 *planned*

- **WS-Beilngries**
  - September 4th-6th 2008

- **WS-Salzgitter**
  - September 27th-30th 2009

- **MSE-Darmstadt**
  - Materials Science & Engineering
  - August 2010

- **Korea Excursion**

- **SFB-Start**
  - July 2007

- **DFG-Evaluation**
  - March 2011

**Time bar**

- 2007
  - 01.07.2007
  - 01.07.2008

- 2008
  - 01.07.2008
  - 01.07.2009

- 2009
  - 01.07.2009
  - today

- 2010
  - 01.07.2010

- 2011
  - 01.07.2011
1. Motivation / Background / General Information
   • Material-Development
   • Method-Development

2. General Information
   • Structure / Participants (PB-, TP-Leiter)

3. Scientific progress / first results
   • Modelling
   • Material processing
   • Evaluation

4. Integrated Graduate School

5. Future plans / Vision
Steel ab initio

1. Motivation / Background / General Information
   • Material-Development
   • Method-Development

2. General Information
   • Structure / Participants (PB-, TP-Leiter)

3. Scientific progress / first results
   • Modelling
   • Material processing
   • Evaluation

4. Integrated Graduate School

5. Future plans / Vision
One supercell $\text{Fe}_{16}\text{Mn}_{16}$ that comprises all 10 kinds of octahedral voids

Random distribution of C?
Random distribution of C?

Enthalpies of different Fe–Mn–C ordering
Effect of Temperature and Chemical Composition on SFE

• *ab initio* techniques
  - e.g. the Density Functional Theory (DFT) to simulate the irregularities in the stacking order of atomic layers
→ Magnetism plays critical role for SFE
- SFE is increased by up to a factor of 2
- Qualitatively agree with experiment
• Temperature effects are important, but…
• Are not strong enough
• Thermal volume expansion plays dominant role
- *ab initio* techniques
  e.g. the Density Functional Theory (DFT) to simulate the irregularities in the stacking order of atomic layers

- Transmission Electron Microscopy (TEM)
  e.g. size of the dislocation splitting width
Stacking Faults at Dislocations
• *ab initio* techniques
e.g. the Density Functional Theory (DFT) to simulate the irregularities in the stacking order of atomic layers

• Transmission Electron Microscopy (TEM)
e.g. size of the dislocation splitting width

• Inference from the experimental data
e.g. exp. observation of TRIP and TWIP mechanisms

• Thermodynamics-based models
e.g. subregular solution model

**Determination of SFE**
Steel *ab initio*

1. Motivation /Background / General Information
   - Material-Development
   - Method-Development

2. General Information
   - Structure / Participants (PB-, TP-Leiter)

3. Scientific progress / first results
   - Modelling
   - Material processing
   - Evaluation

4. Integrated Graduate School

5. Future plans / Vision
Fe-Mn-C alloy selection
Process Chain of Material Production

Problems encountered
- Inhomogeneities in the Mn and C content in the micro scale (cast state)
- Strong oxidation during heating and annealing caused inrolled scale

Problems solved
- Approved homogenization strategy by forging, annealing and hot rolling
- Descaler to reduce the oxidation layer before hot rolling
High purity alloy I
Steel *ab initio*

1. Motivation / Background / General Information
   - Material-Development
   - Method-Development

2. General Information
   - Structure / Participants (PB-, TP-Leiter)

3. Scientific progress / first results
   - Modelling
   - Material processing
   - Evaluation

4. Integrated Graduate School

5. Future plans / Vision
Strain hardening behaviour
Interpretation strain hardening rate

Stage A (similar to stage III)
Stage B (primary twinning)
Stage C (Decreasing rate of primary twinning)
Stage D (Twin intersections)

Microstructure – ECCI images


Deformation Twins in high Mn steels
Structure of the model

Based on microstructural observations, the model takes dislocation cells and twinning into account.

10% of the microstructure is dense dislocation walls (DDWs), but no size is specified. The volume fraction of DDWs does not change.

The average twin thickness is 15nm.

Different twin systems are not treated differently, only a global twin volume fraction is considered.
• Microstructure must be described by state variables
  – Chosen state variables are dislocation densities and twin volume fraction
    \[ \rho_{wa} \quad \rho_{cell} \quad \rho_{morb} \quad \dot{f}_{tw} \]

• Evolution of those state variables describes microstructure evolution
  – Evolution of the dislocation densities from multiplication and recovery rates
    \[ \dot{\rho}_t = \dot{\rho}_{wa} + \dot{\rho}_f + \dot{\rho}_m \]
  – Evolution of the twin volume fraction by nucleation
    \[ \dot{f}_t = (f_t^s \cdot \frac{a}{w} \cdot f_t^t)_w \cdot \dot{N} \cdot V \]
• Mean Free Path (MFP) of dislocations governs hardening behavior
\[ \frac{1}{L_e} = \frac{i_c}{L_c} + \frac{i_w}{L_w} + \frac{1}{d_{gr}} + \frac{i_{tw}}{L_{tw}} \]

• Extended by incorporation of twinning
\[ L_{tw} = \frac{(1 - f_{tw})d_{tw}}{f_{tw}} \]

• Evolution of twin volume fraction
\[ \dot{f}_t = (f_t^s \cdot \frac{a}{f_t^t}) \tilde{N}V \]

• Can be directly included in FE code

Simplified statistical model
Experiment versus Simulation I: Without twinning

True Stress-True Strain / Hardening Curve

- Hardening Simulation
- True Stress-True Strain Simulation
- True Stress-True Strain Experiment
- Hardening Experiment

\( \frac{d\sigma}{d\varepsilon} (\text{Pa}) \)

\( \sigma (\text{Pa}) \)

\( \varepsilon \)
Experiment versus Simulation II: With twinning, saturation 10%
Experiment versus Simulation III: With twinning, saturation 20%
Thermographic plot of a tensile test
Temperatur dependency during tensile test
Schematic stress-strain curve

- Strain hardening = formability / safety
- Damage evolution = formability / safety

Well/partly known vs. new topic
The void nucleation site in TRIP-steels is strongly dependent on the austenite stability.

<table>
<thead>
<tr>
<th>Austenite stability</th>
<th>Inclusion</th>
<th>Martensite</th>
</tr>
</thead>
<tbody>
<tr>
<td>high</td>
<td>+ +</td>
<td></td>
</tr>
<tr>
<td>medium</td>
<td>+</td>
<td>+</td>
</tr>
<tr>
<td>low</td>
<td></td>
<td>+ +</td>
</tr>
</tbody>
</table>
Damage development – schematically
Steel *ab initio*

1. **Motivation /Background / General Information**
   - Material-Development
   - Method-Development

2. **General Information**
   - Structure / Participants (PB-, TP-Leiter)

3. **Scientific progress / first results**
   - Modelling
   - Material processing
   - Evaluation

4. **Integrated Graduate School**

5. **Future plans / Vision**
Steel *ab initio*

- Doctorate Seminars, including lectures (monthly)
- Workshops with scientific coaches (annually)
- Korea Workshop
- You-tube-Lecture
Steel *ab initio*

1. Motivation /Background / General Information
   - Material-Development
   - Method-Development

2. General Information
   - Structure / Participants (PB-, TP-Leiter)

3. Scientific progress / first results
   - Modelling
   - Material processing
   - Evaluation

4. Integrated Graduate School

5. Future plans / Vision
Steel *ab initio*

- Concept for 2nd period
- New topics (e.g. hydrogen effects)
- Alloying elements (e.g. Aluminium, Silicon)
- New SFB members (RWTH, MPI)
- Co-operation network (international)
- Transfer projects (industrial partners)
SFB 761 „Stahl ab initio“

Quantum mechanics guided design of new Fe based materials