SFB 761 „Steel – ab initio“

Mechanism-Oriented Materials Selection
High Mn Systems – New Opportunities

ECO-Index of Steels with High Mn Content

HMS: High Mn Steels
AHSS: Advanced High-Strength Steels
TRIP: Transformation Induced Plasticity
TWIP: Twinning Induced Plasticity
MBIP: MicroBand Induced Plasticity
Stacking Fault Energy (SFE) defines the active modes of plasticity: dislocation glide, TRIP, TWIP, etc.
Thermodynamics-Based Approach

\[ \gamma_{fcc} = 2 \rho \Delta G^{\gamma \rightarrow \varepsilon} + 2 \sigma^{\gamma / \varepsilon} \]

CALPHAD \hspace{2cm} ab-initio

Mechanism Maps
Mechanism Maps

Computational Pattern
Maps of Gibbs Free Energy

\[ \gamma_{fcc} = 2\rho \left( \Delta G^{\gamma \rightarrow \varepsilon} \right) + 2\sigma^{\gamma/\varepsilon} \]

**SGTE Database**
(Scientific Group Thermodata Europe)

**Kaufman Database**

TRIP
Different Types of SFE Maps

$$\gamma_{fcc} = 2\rho \Delta G^{\gamma \rightarrow \varepsilon} + 2\sigma^{\gamma / \varepsilon}$$

Mechanism Maps

[Graph showing TWIP and TRIP phases with Manganese content and Carbon content on the x-axis, Tempereature on the y-axis, and 300 K, 0.6 wt.% C indicated.]
Stacking Fault Energy Calculator

(Regular Solution Thermodynamic Model)
Checking the Accuracy of Design

Deformation Response

Manganese content [wt.\%] vs. Carbon content [wt.\%] diagram showing the transition from TRIP to TWIP at 300 K.
Checking the Accuracy of Design

Deformation Response
Checking the Accuracy of Design

TRIP/TWIP Steel after deformation

Manganese content [wt.%] vs Carbon content [wt.%]

Phase Fraction
- Iron - Alpha: 0.000
- Iron - Gamma: 0.786
- Iron - Epsilon: 0.214

After deformation

TRIP/TWIP Steel
Work Hardening Rate

Deformation Response
Mechanical Properties

Deformation Response

UTS: Ultimate Tensile Strength
El.: Elongation to fracture

TRIP
TWIP

AHSS

15 mJ/m²
27 mJ/m²
Jerky Flow

Flow Behaviour in Fe-Mn-C System

Fe – 22 wt.% Mn – 0.6 wt.% C
Thermography Investigation

- The film is 50 times faster than the actual test!

Low Strain Rate

Flow Behaviour in Fe-Mn-C System
The film is 4 times faster than the actual test!
SFE Variations

Flow Behaviour in Fe-Mn-C System
Flow Behaviour in Fe-Mn-C System
Stage #1:
Acceleration of cross-head of tensile machine till the onset of plastic flow
Stage #2: Pronounced strain hardening
Stage #2: Pronounced strain hardening
Stage #2:

Pronounced strain hardening

Significant dislocation interaction
Stage #3: 
Non-pronounced serrated flow
Stage #3:  
Non-pronounced serrated flow  
Onset of deformation twinning  

SRS > 0 or SRS < 0  

SRS: Strain Rate Sensitivity
Stage #3:
Non-pronounced serrated flow
Onset of deformation twinning

SRS > 0 or SRS < 0

SRS: Strain Rate Sensitivity

Flow Behaviour in Fe-Mn-C System
Stage #4:

Pronounced serrated flow

SRS < 0 (nSRS)

nSRS: negative Strain Rate Sensitivity
Stage #4:
Pronounced serrated flow

SRS <0 (nSRS)

nSRS: negative Strain Rate Sensitivity

Flow Behaviour in Fe-Mn-C System
Stage #4:

- Pronounced serrated flow
- Heavy twinning and twins intersection
Increasing effect of aluminum on SFE
TWIP steels resistant to hydrogen attack
Decrease in density of sheet products
Changes of twins’ internal structures


Aluminum in High Mn Systems

- Carbide formation and enhancement of planar glide
- Microband formation and the resultant plasticity

Quantum-mechanics guided design
of new Fe-based materials

THANK YOU!