Prediction of Deformation Mechanisms using Thermodynamics-Based SFE Maps in High-Mn Steels Systems

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• Main Targets
• Background of Research
• Thermodynamics-Based Fundamentals
• Mechanism Maps
  • Methodology
  • Composition – Composition SFE Maps
  • Composition – Temperature SFE Maps
  • Maps of $\Delta G^{\gamma \rightarrow \varepsilon}$
  • Map of $T_0^{\gamma \rightarrow \varepsilon}$
• Sample Thermodynamics-Based Designs
  • Success Story
  • Drawbacks
• Summary and Outlook
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• Summary and Outlook
- Building up models to assist and to facilitate steel design in high-Mn steels systems
- Adjustment of process parameters like working-temperature to activate twinning mechanism (TWIP) or strain-induced martensite formation (TRIP)
- Steel Design in Fe-Mn-C system
- Application of the developed techniques in Fe-Mn-Al-C and other highly-alloyed austenitic systems for a fast and accurate design
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Fe-Mn-Al-C
Steels
Fe-Mn-Al-C System
• A stacking fault $ABCBCABC$ may be regarded as two overlapping twin boundaries $CBC$ and $BCB$ across which the next nearest neighboring planes are wrongly stacked.

• In fcc crystals any sequence of three atomic planes not in the ABC or CBA order is a stacking violation and is accompanied by an increased energy contribution (SFE).

• The SFE is assumed to change the ability of a dislocation in a crystal to glide onto an intersecting slip plane.

• When the SFE is low, the mobility of dislocations in a material decreases.

Source:
• R. E. Smallman, R. J. Bishop: Modern physical metallurgy and materials engineering, Reed 1999.
• http://en.wikipedia.org/wiki/Stacking-fault_energy
The equilibrium separation of two partial dislocations is calculated by:

\[ d = \frac{\mu a^2}{24\pi\gamma_{SF}} \]

from which it can be seen that the width of the stacking fault ‘ribbon’ is inversely proportional to the value of the stacking fault energy, \( \gamma_{SF} \), and also depends on the value of the shear modulus, \( \mu \).
Activation of different deformation mechanisms based on the SFE value:

- **TRIP + TWIP**
  - SFE < 18-20 mJ/m²
- **Pure Slip**
  - 25-60 mJ/m²
  - 25-80 mJ/m²

SFE [mJ/m²]
Schumann → microstructure based

Scott and Allain → SFE approximation based on Schumann

V. H. Schumann, Neue Hütte 17 (1972) 605-609
C. Scott et al., Rev. Met. 103 (2006) 6, 293-302
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• **ab initio** techniques
e.g. the Density Functional Theory (DFT) to simulate the irregularities in the stacking of atomic layers

• Transmission Electron Microscopy (TEM)
e.g. variations in the size of the dislocation nodes

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

• Thermodynamics-based models
e.g. subregular solution model
• *ab initio* techniques
  e.g. the Density Functional Theory (DFT) to simulate the irregularities in the stacking of atomic layers

• Transmission Electron Microscopy (TEM)
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• Inference from the experimental data
  e.g. observation of TRIP and TWIP mechanisms in practice

• Thermodynamics-based models
  e.g. subregular solution model
\[ \gamma_{fcc} = 2 \rho \Delta G^{\gamma \rightarrow \varepsilon} + 2 \sigma^{\gamma / \varepsilon} \]

\[ \Delta G^{\gamma \rightarrow \varepsilon} = X_{Fe} \Delta G_{Fe}^{\gamma \rightarrow \varepsilon} + X_{Mn} \Delta G_{Mn}^{\gamma \rightarrow \varepsilon} + X_{C} \Delta G_{C}^{\gamma \rightarrow \varepsilon} + X_{Fe} X_{Mn} \Delta \Omega_{FeMn}^{\gamma \rightarrow \varepsilon} + X_{Fe} X_{C} \Delta \Omega_{FeC}^{\gamma \rightarrow \varepsilon} + 
X_{Mn} X_{C} \Delta \Omega_{MnC}^{\gamma \rightarrow \varepsilon} + \Delta G_{mg} \]

\[ \Delta G_{Fe}^{\gamma \rightarrow \varepsilon} (J/mol) = -2243.38 + 4.309T \]
\[ \Delta G_{Mn}^{\gamma \rightarrow \varepsilon} (J/mol) = -1000.00 + 1.123T \]
\[ \Delta G_{C}^{\gamma \rightarrow \varepsilon} (J/mol) = -22166 \]
\[ \Delta \Omega_{FeMn}^{\gamma \rightarrow \varepsilon} (J/mol) = 2180 + 532(X_{Fe} - X_{Mn}) \]
\[ \Delta \Omega_{FeC}^{\gamma \rightarrow \varepsilon} (J/mol) = 42500 \]
\[ \Delta \Omega_{MnC}^{\gamma \rightarrow \varepsilon} (J/mol) = 26910 \]
\[ \sigma^{\gamma / \varepsilon} (mJ/m^2) \approx 10 \]
\[ \gamma_{fcc} = 2 \rho \Delta G^\gamma \rightarrow \varepsilon + 2 \sigma^{\gamma / \varepsilon} \]

- **reliable databases**
- **empirical or ab-initio calculations**
  (no global model available!)

5 – 15 mJ/m\(^2\)
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Computational Pattern
Gibbs Free Energy

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

Methodology

Stacking Fault Energy
Composition – Composition Maps

- **Pure Dislocation Glide**
- **TWIP**
- **TRIP**
- **Fe-Mn-C 296 K**
- **Fe-Mn-C 373 K**
- **Aluminum content: 3.0 wt.%**

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

\[ \Delta G^{\gamma \rightarrow \varepsilon} = X_{Fe} \Delta G_{Fe}^{\gamma \rightarrow \varepsilon} + X_{Mn} \Delta G_{Mn}^{\gamma \rightarrow \varepsilon} + X_{C} \Delta G_{C}^{\gamma \rightarrow \varepsilon} + 
X_{Fe} X_{Mn} \Delta \Omega_{FeMn}^{\gamma \rightarrow \varepsilon} + X_{Fe} X_{C} \Delta \Omega_{FeC}^{\gamma \rightarrow \varepsilon} + X_{Mn} X_{C} \Delta \Omega_{MnC}^{\gamma \rightarrow \varepsilon} + \Delta G_{mg} \]

\[ \Delta G^{\gamma \rightarrow \varepsilon} = 0 \quad \Rightarrow \quad T_0^{\gamma \rightarrow \varepsilon} \]
\( \gamma \rightarrow \varepsilon \) Borderline of Transformation in Fe-Mn-Al-C System

Borderline of \( \Delta G_{\gamma \rightarrow \varepsilon} = 0 \)
Borderline of transformation in Fe-Mn-Al-C system

\[ \gamma \rightarrow \varepsilon \]

\[ \Delta G_{\gamma \rightarrow \varepsilon} = 0 \]

~ 150,000 calculated points!
Building a model for $T_0^{\gamma\rightarrow\varepsilon}$
sigmoidal logistic function

Equivalent effect on the TRIP \( \rightarrow \) TWIP transition boundary

0.2 wt.% C = 1.0 wt.% Al

Building a model for \( T_0^{\gamma \rightarrow \epsilon} \)
\[ T_{0}^{\gamma \to \varepsilon} (Mn) = \frac{a(x)}{1 + e^{-b(x)(Mn-c(x))}} \]

\[ x = Al + 5 \, C \]

\( (Mn, Al \text{ and } C \text{ in wt. } \%) \)
$T_{0}^{\gamma \rightarrow \varepsilon}(Mn) = \frac{a(x)}{1 + e^{-b(x)(Mn-c(x))}}$

$x = Al + 5 C$

(Mn, Al and C in wt. %)

$a(x) = -36.21581 \, x + 436.29441 \pm a'(x)$

$b(x) = -0.19131 \, x - 0.56821 \pm b'(x)$

$c(x) = -3.08868 \, x + 31.18241 \pm c'(x)$

Building a model for $T_{0}^{\gamma \rightarrow \varepsilon}$
\[ T_{0}^{\gamma \rightarrow \epsilon}(Mn) = \frac{a(x)}{1 + e^{-b(x)(Mn-c(x))}} \]

\[ x = Al + 5C \]

(Mn, Al and C in wt. %)

\[ a(x) = -36.21581x + 436.29441 \pm a'(x) \]
\[ b(x) = -0.19131x - 0.56821 \pm b'(x) \]
\[ c(x) = -3.08868x + 31.18241 \pm c'(x) \]

\[ a'(x) = 0.07457x^2 - 0.5546x + 2.32626 \]
\[ b'(x) = -0.0006875x^2 + 0.00527x + 0.01188 \]
\[ c'(x) = 0.0025x^2 - 0.014x + 0.0351 \]
The diagram shows the map of $T_0^{\gamma \rightarrow \epsilon}$ with the carbon content on the x-axis and the manganese content on the y-axis. The shaded area indicates the region where the $\gamma \rightarrow \epsilon$ transformation is not thermodynamically feasible. The Schumann line is marked on the diagram.
Map of $\Delta T = T_{\text{testing}} - T_{0}^{\gamma \rightarrow \varepsilon}$

- $T_{\text{testing}} : 300 K$
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Drawback?
iso-SFE designs?
Thermodynamics-based steel design has a potential to accelerate the materials selection in highly alloyed austenitic systems.

Further investigations are required to build-up models for the interfacial energies to be able to accurately estimate the SFE value.

Attention to the effects of interstitial and substituional alloying content beside mechanism maps might be required.

High-Mn TRIP steel can be considered as an alternative for the high-Mn TWIP steel with a same UTS level but a completely different strain-hardening behavior.
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Thank you!