Flow curve and failure modelling for high-Mn steels on a microstructural scale

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• Material characterization and mechanical properties
• Fracture and failure
• RVE modelling
• Material modelling
• Results and summary
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Chemical Composition

<table>
<thead>
<tr>
<th>Grade</th>
<th>Fe</th>
<th>C</th>
<th>Mn</th>
<th>Si</th>
<th>P</th>
<th>S</th>
<th>Cr</th>
<th>Ni</th>
<th>Al</th>
<th>N</th>
<th>Nb</th>
<th>V</th>
</tr>
</thead>
<tbody>
<tr>
<td>TWIP 900</td>
<td>76,9</td>
<td>0,31</td>
<td>22,28</td>
<td>0,12</td>
<td>0,015</td>
<td>0,001</td>
<td>0,243</td>
<td>0,014</td>
<td>0,003</td>
<td>0,012</td>
<td>0,014</td>
<td>0,018</td>
</tr>
<tr>
<td>TWIP 1000</td>
<td>76,3</td>
<td>0,58</td>
<td>22,48</td>
<td>0,25</td>
<td>0,019</td>
<td>0,001</td>
<td>0,074</td>
<td>0,030</td>
<td>0,004</td>
<td>0,009</td>
<td>0,019</td>
<td>0,219</td>
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<tr>
<td>TRIP 700</td>
<td>96,2</td>
<td>0,18</td>
<td>1,77</td>
<td>0,04</td>
<td>0,014</td>
<td>0,007</td>
<td>0,031</td>
<td>0,036</td>
<td>1,610</td>
<td>0,011</td>
<td>0,001</td>
<td>0,003</td>
</tr>
</tbody>
</table>

Mechanical Properties

<table>
<thead>
<tr>
<th>Grade</th>
<th>$R_{p0.2}$ [MPa]</th>
<th>$R_m$ [MPa]</th>
<th>$A_u$ [-]</th>
<th>TEL [-]</th>
</tr>
</thead>
<tbody>
<tr>
<td>TWIP 900</td>
<td>310</td>
<td>900</td>
<td>0,37</td>
<td>0,39</td>
</tr>
<tr>
<td>TWIP 1000</td>
<td>380</td>
<td>1010</td>
<td>0,38</td>
<td>0,4</td>
</tr>
<tr>
<td>TRIP 700</td>
<td>460</td>
<td>730</td>
<td>0,23</td>
<td>0,29</td>
</tr>
</tbody>
</table>

Chemical composition, mechanical properties and strain hardening of investigated steels
Initial and deformed structure of high-Mn steels

**TWIP 1000**
Initial: Grain size: 2µm
Deformed: Twin lamella distance < 100 nm

**TWIP 900**
Initial: Grain size: 100µm
Deformed: Twin lamella distance < 100 nm

**TRIP 700**
Initial: Grain size: 5µm
Deformed: Twin lamella distance < 100 nm
Microstructure development and flow curves of TWIP 900

- EBSD

Austenite: 68 %
ε-Martensite: 64 %
Other: 2 %

Temperature: 173 K, 273 K, 373 K
SFE [mJ/m²]: 17, 26, 42

Twin fraction: 5 %, 23 %, 44 %

true strain [-]
true stress [MPa]
As received
Grain size: 2 µm

<table>
<thead>
<tr>
<th>Position [-]</th>
<th>Mn [wt. %]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Min.</td>
</tr>
<tr>
<td></td>
<td>21.47</td>
</tr>
</tbody>
</table>

Measurement of manganese content in 22Mn0.6C TWIP steel (TWIP 1000)
Measurement of manganese content in 22Mn0.6C TWIP steel (TWIP 900)

Annealed: 1030 °C / 30 min
Grain size: 100 µm

Position [-] 1 2 3 4 5

Mn [wt. %]
Min. [wt. %] 21.31
Max. [wt. %] 24.58
Mean [wt. %] 22.64
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Fractography of a 22Mn0.6C steel at different temperatures and for varying grain size
- Plot of void size, yield strength, tensile strength, total elongation and SFE versus temperature
- Void size measurement by digital image analysis
In-situ bending test of pre-strained tensile specimens

- In-situ bending device
- Max. force 5000N
- Max. displacement 15mm
- Temperature up to 800 °C

SEM

Sample

Cathode

Force

Sample
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
- Coarseness due to twinning
- Fracture occurs on surface at shear bands
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Multiscale modelling

- Modelling the macroscopic structure
- Assignment of RVE to integration point in the macroscopic model
- Definition of the boundary conditions for the RVE according the macroscopic strain state
- Computation on microscale
- Determination of the macroscopic stress state by homogenization of the RVE
- RVE – Generator (based on mesh creation)
- Constitutive material model (TWIP + TRIP) (Based on dislocation evolution)
- Incorporation of grain size and orientation (Taylor-factor)
- Implementation of failure and fracture (CZM)
RVE generation by continuous 3D Voronoi diagram calculation (voro++)

Mesh generation by Gmsh

Discrete and continuous Voronoi diagram with grains size and taylor factor distribution

Discrete RVE with cubic mesh elements and 200 grains

Continuous RVE with tetrahedral mesh elements and 200 grains
Overview

- Material characterization and mechanical properties
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Material model for high-Mn steels with TRIP and TWIP effect
Stacking fault energy [mJ/m²]:
\[ \Gamma = 2\rho \Delta G^{\gamma\rightarrow\varepsilon} + 2\sigma^{\gamma/\varepsilon} \]

\[ \Delta G^{\gamma\rightarrow\varepsilon} \] Free energy

\[ \sigma^{\gamma/\varepsilon} \] Interfacial energy

\[ \rho \] Molar surface density along {111} planes

\[ \Delta G^{\gamma\rightarrow\varepsilon} = X_{Fe}\Delta G^{\gamma\rightarrow\varepsilon}_{Fe} + X_{Mn}\Delta G^{\gamma\rightarrow\varepsilon}_{Mn} + X_{Al}\Delta G^{\gamma\rightarrow\varepsilon}_{Al} + X_{C}\Delta G^{\gamma\rightarrow\varepsilon}_{C} + X_{Fe}X_{Mn}\Delta \Omega^{\gamma\rightarrow\varepsilon}_{FeMn} + X_{Fe}X_{Al}\Delta \Omega^{\gamma\rightarrow\varepsilon}_{Fe} + X_{Fe}X_{C}\Delta \Omega^{\gamma\rightarrow\varepsilon}_{FeC} + X_{Mn}X_{C}\Delta \Omega^{\gamma\rightarrow\varepsilon}_{MnC} + \Delta G^{\gamma\rightarrow\varepsilon}_{mag} \]

Stress-strain curve of austenite
\[ \sigma = \sigma_0 + \alpha MG b \sqrt{\rho} \]

Dislocation evolution
\[ \frac{d\rho}{Md\varepsilon} = \frac{1}{bd} + \frac{k}{b} \sqrt{\rho} - f \rho \]

Austenite grain size evolution:
\[ d = d_{init}\sqrt[3]{1 - f} \]

Dynamic grain size refinement by evolution of twin or \( \varepsilon \)-martensite volume fraction \( f \)

Critical shear stress for twinning

\[ \tau_{cr} = \frac{\gamma_{sfe}}{b} + \frac{Gb}{D} \]

Nucleation probability

\[ N_{prob} = \exp\left(-\left(\frac{\tau_{cr}}{\tau_{ext}}\right)^s\right) \]

Nucleation rate

\[ N_{rate} = N_{rate_0} \cdot N_{prob} \]

Volume of new twin

\[ N_{vol} = \frac{1}{6}\pi d_{twin} l_{twin}^2 \]

Twin volume fraction

\[ f_{twin} = (f_{twin_{sat}} - f_{twin}) N_{rate} N_{vol} \dot{\varepsilon} \]

Source: I. Gutierrez et al: The effect of grain size and grain orientation on deformation twinning in a Fe–22 wt.% Mn–0.6 wt.% C TWIP steel (2010)
S. Mahajan and G. Y. Chin: Formation of deformation twins in f.c.c crystals (1973)
D. Steinmetz (2010)
Material model for martensitic phase transformation

\[
\sigma_{\varepsilon} = \sigma_0 + \alpha \mu M \sqrt{b} \sqrt{1 - e^{\left(-M f \varepsilon\right) f L}}
\]

Yield strength of martensite
\[
\sigma_0 = 413 + 1.72 \times 1000 (\text{wt.\%C})^{1/2}
\]

\(\varepsilon\)-martensite volume fraction
\[
f_\varepsilon = (1 - e^{-\alpha \varepsilon})^n
\]

\(\alpha'\)-martensite volume fraction
\[
f_{\alpha'} = 1 - e^{-\beta f_\varepsilon}
\]

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Numerical calculation of twin and $\varepsilon$-martensite volume fraction
Comparison of different grain size and temperatures

TWIP 1000
Grain size: 2 µm
Strain rate: 0.001 1/s

TWIP 900
Grain size: 100 µm
Strain rate: 0.001 1/s

Comparison of experimentally measured and calculated flowcurves.
Fracture evolution by means of Cohesive Zone Elements

- Cohesive zone model for 22Mn0.6C (233 K) (cleavage fracture is dominant).
- Cohesive elements are defined in the overall midplane of the RVE model.
- Local structure analysis on steels with varying chemical composition
- RVE generation based on microstructure
- Material model development regarding SFE and implementation
- Parameter studies and verification

Damage model (CZM)

Material model

Mechanism map SFE

Microstructure
Thank you for your attention!
Description of cleavage failure by means of a Cohesive Zone Model

The dissipated energy of the cohesive elements serves as a failure criterion:

\[ \Gamma_0 = \int_0^{\delta_0} T(\delta) d\delta \]

- \( T \) – Traction
- \( \delta \) – Separation, opening of the cohesive
- \( \Gamma \) – Cohesive energy