A COMPUTATIONAL APPROACH FOR DESIGNING TRIP STEELS

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Alloy Design

Genetic Algorithms

Experimental Validation

Tests

Property

Microstructure

Composition

Computational Design
Experimental Results - Fe-0.32C-1.42Mn-1.56Si

![Graph showing true stress vs. true strain for different treatments: As-cast, 950°C ECAEed 2 passes route C, 950°C ECAEed 2 passes route C+, Not optimized two-step heat treatment, and Optimized Two-step heat treatment.](image-url)
Outline

• Motivations

• CALPHAD-based Models

• Mechanical Models
  ➢ Swift Model
  ➢ Irreversible Thermodynamics

• Genetic Algorithms

• Artificial Neural Network

• Conclusion
The Properties of TRIP Steel

Why TRIP Steel
- Transformation Induced Plasticity
- Martensitic transformation during plastic deformation contributes to overall ductility

How to make TRIP steels
- Select chemical composition properly
- Apply two-step heat treatment to manage the carbon content in austenite

Target
- Maximize TRIP effect of the low alloying addition TRIP steel

Key
- Stabilize austenite against the martensitic transformation during heat treatment
- Suppress the formation of cementite

Zhu, Acta Mat., 2012
Two-step heat treatment:

1. Inter-critical annealing (IA)
2. Bainite isothermal transformation (BIT)
3. Final cooling to room temperature

Zhu, Acta Mat., 2012
Two-step heat treatment: (1) inter-critical annealing (IA)

Li, Acta Mat., 2012
Li, Acta Mat., 2013
Two-step heat treatment: (1) inter-critical annealing (IA) (2)-(3) bainite isothermal transformation (BIT) (3)-(4) final cooling to room temperature

Li, Acta Mat., 2012
Li, Acta Mat., 2013
Displacive Bainitic Transformation

- The Gibbs free energies of bainitic ferrite and austenite are equal at $T_0$.
- 400 J/mole of the strain energy is considered for bainitic transformation as $T_0'$.
- The non-homogeneous C-distribution sustains the bainitic transformation.
- The curve is fitting based on database TCFE6 V6.2
- The empirical data is obtained from: Chang et al., Met. Mat. Tran. A, 1999 and Zhao et al., J. Mat. Sci., 2001
“During the growth some carbon diffuses out of the ferrite grains into the surrounding austenite matrix. The higher the temperature of formation, the freer the ferrite is of supersaturated carbon.”

– Zener, 1912
Heterogeneous Carbon Distribution (1)
Heterogeneous Carbon Distribution (2)

DC $>>$ df

DC $<<$ df
Heterogeneous Carbon Distribution (3)

Caballero et al., 2011
Two-step heat treatment: (1) inter-critical annealing (IA) (2)-(3) bainite isothermal transformation (BIT) (3)-(4) final cooling to room temperature

Li, Acta Mat., 2012
Li, Acta Mat., 2013
Mechanical Properties

Swift Model

\[
\sigma_i = K_i (1 + \varepsilon_{0,i} \varepsilon)^{n_i}
\]

\[
\sigma = \sum_i \sigma_i Vf_i
\]

\[
\sigma = \sigma_A + (\sigma_B - \sigma_A) \frac{w_C^\gamma - 1.25}{0.25}
\]

### Composition and micro-structure in tensile tests

<table>
<thead>
<tr>
<th></th>
<th>(w_C)</th>
<th>(w_{Mn})</th>
<th>(w_{Si})</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>0.29</td>
<td>1.42</td>
<td>1.41</td>
</tr>
<tr>
<td>B</td>
<td>0.29</td>
<td>1.42</td>
<td>1.41</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>(Vf_{Fe})</th>
<th>(Vf_{Bai})</th>
<th>(Vf_{Aus})</th>
<th>(Vf_{Mar})</th>
<th>(w_C^\gamma)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>55</td>
<td>28</td>
<td>17</td>
<td>0</td>
<td>1.25</td>
</tr>
<tr>
<td>B</td>
<td>55</td>
<td>33</td>
<td>12</td>
<td>0</td>
<td>1.5</td>
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</tbody>
</table>

### Mechanical Properties

<table>
<thead>
<tr>
<th>Phase</th>
<th>(K_i), MPa</th>
<th>(\varepsilon_{0,i})</th>
<th>(n_i)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Austenite</td>
<td>720</td>
<td>62</td>
<td>0.3</td>
</tr>
<tr>
<td>BCC</td>
<td>475</td>
<td>55</td>
<td>0.27</td>
</tr>
<tr>
<td>Martensite</td>
<td>2000</td>
<td>800</td>
<td>0.005</td>
</tr>
</tbody>
</table>

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<tr>
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<th>(K_i), MPa</th>
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<th>(n_i)</th>
</tr>
</thead>
<tbody>
<tr>
<td>B</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Austenite</td>
<td>1130</td>
<td>80</td>
<td>0.2</td>
</tr>
<tr>
<td>BCC</td>
<td>720</td>
<td>50</td>
<td>0.175</td>
</tr>
<tr>
<td>Martensite</td>
<td>2000</td>
<td>800</td>
<td>0.005</td>
</tr>
</tbody>
</table>
Optimum Heat Treatment for Fe-0.32C-1.42Mn-1.56Si

<table>
<thead>
<tr>
<th>$T_{IA}$</th>
<th>$T_{BIT}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>943 - 1142</td>
<td>350 - 943</td>
</tr>
</tbody>
</table>

The temperature domains (Kelvin) for optimizing the heat treatment for Fe-0.32C-1.42Mn-1.56Si

Case 1

Case 2

Case 3
The Predictions for Case 1

Vf(Fer)

Vf(Bai)

Vf(Aus)

Vf(Mar)
The Predictions for Case 1

1. Strain, %
2. Strength, MPa
3. WTN, MPa%
The Predictions for Case 2

Vf(Fer)

Vf(Bai)

Vf(Aus)

Vf(Mar)
The Predictions for Case 2

(1) Strain, %

(2) Strength, MPa

(3) WTN, MPa%
The Predictions for Case 3

In $T_0'$ calculations, for most of the microstructures the predicted retained austenite is less than 5%. Therefore, these diagrams include all the predicted microstructures.
Optimum Heat Treatment for Maximizing Toughness

Experiments
Alloy Design Process

- **Genetic Algorithms**
- **Experimental Validation**
  - Tests
- **Property**
- **Microstructure**
- **Composition**

**Computational Design**
Genetic Algorithms - Schema
Optimum Composition and Heat Treatment

Composition, wt%; Temperature, Kelvin

<table>
<thead>
<tr>
<th>$W_C$</th>
<th>$W_{Mn}$</th>
<th>$W_{Si}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1 - 0.5</td>
<td>0.5 - 2.5</td>
<td>0.8 - 1.5</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$T_{IA}$</th>
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</tr>
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<td>943 - 1142</td>
<td>350 - 943</td>
</tr>
</tbody>
</table>

1. 6 bits memory for each variable
2. $V_{f_{Aus}} > 5$
3. Total alloying addition is less than 4 wt%
4. 10 individuals in one generation, 1,000 generations
5. Full equilibrium after IA treatment is considered
6. $T_0$ and para $\gamma - \theta$ concepts are utilized
The Predicted Fitness as Function of Mechanical Properties

Objective Function

\[ f(x) = \frac{Vf_{Aus}}{w_C^\gamma (0.01 + Vf_{Mar})} \]
Chemical Composition vs Mechanical Properties

(1) $w_C$

(2) $w_{Mn}$

Fe-0.32C-1.42Mn-XSi

(3) $w_{Si}$
The Search in 6 Components, 2 Temperatures Domain

<table>
<thead>
<tr>
<th>$w_C$</th>
<th>$w_{Mn}$</th>
<th>$w_{Si}$</th>
<th>$w_{Al}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1 - 0.5</td>
<td>0.5 - 2.5</td>
<td>0.8 - 1.5</td>
<td>0.0 - 2.0</td>
</tr>
<tr>
<td>$w_{Cr}$</td>
<td>$w_{Ni}$</td>
<td>$T_{IA}$</td>
<td>$T_{BIT}$</td>
</tr>
<tr>
<td>0.0 - 1.33</td>
<td>0.0 - 2.0</td>
<td>943 - 1142</td>
<td>350 - 943</td>
</tr>
</tbody>
</table>

Composition, wt%; Temperature, Kelvin

1. 6 bits memory for each variable
2. $Vf_{Aus} > 5%$
3. Total alloying addition is less than 4 wt%
4. 10 individuals in one generation, 10,000 generations
5. Full equilibrium after IA treatment is considered
6. $T_0$ and para $\gamma - \theta$ concepts are utilized
Predicted Fitness as Function of Mechanical Properties

The predicted mechanical properties of Fe-C-Mn-Si-Al-Cr-Ni and Fe-C-Mn-Si alloys
Summary

Composition Selection

C Mn Si Al Ni Cr

Genetic Algorithm

CALPHAD Method

Micro-Structure

Mechanical Properties

Mechanical Model based on Irreversible Thermodynamics
During the isothermal plastic deformation, the energy dissipation, $dE$ can be attributed to (1) the exchange of the energy with the environment, $dQ$; (2) energy consumption by dislocation variation, $dW_E$

$$dE = TdS = \frac{Cb}{l}d\tau = dQ + dW_E$$
Plastic Deformation Model – cont. 1

- By energy conservation, $dQ$ can be calculated

$$dQ = dU - dW_M$$

- Because of the dislocation: (1) **Generation**, $dW_{ge}$; (2) **Glide**, $dW_{gl}$; (3) **Annihilation**, $dW_{an}$

$$dW_E = W_{ge} + W_{gl} + W_{an}$$

The energy dissipation can be estimated as:

$$dE = \frac{1}{2} \mu b^2 d\rho^+_{in} + \tau bld \rho^+_{in} + \frac{1}{2} \mu b^2 d\rho^-_{in} + \frac{1}{2} \mu b^2 d\rho_{in} - \tau_{in} d\varepsilon$$
To estimate the shear stress ($\tau$), several mechanisms are taken into account:

$$\tau = \tau_0 + \tau_s + \tau_{H-P} + \sqrt{\tau_{in}^2 + \tau_p^2}$$

$\tau_0$: Peierls force [Irvine1969; Varin1988; Zhao 2007]

$\tau_s$: solid-solution strengthening [Irvine1969; Varin1988; Zhao 2007]

$\tau_{H-P}$: Hall-Petch effect [Irvine1969; Varin1988; Zhao 2007]

$\tau_{in}$: dislocation strengthening inside the grain

$\tau_p$: precipitation strengthening
This energy dissipation is also related to (1) the hardness parameter \((\sigma^*)\), (2) flow stress \((\tau)\), and (3) strain rate \((\dot{\gamma})\). It is proposed:

\[
TdS = \frac{Cb}{l} d\tau \\
= \frac{1}{2} \mu b^2 d\rho^+_in + \tau bld\rho^+_in + \frac{1}{2} \mu b^2 d\rho^-_in + \frac{1}{2} \mu b^2 d\rho^-_in - \tau_in d\varepsilon
\]

\[
d\rho^-_in = \frac{n_0}{\dot{\gamma}} \exp \left( - \frac{\Delta G}{kT} \right) \rho^-_in d\gamma
\]
Stress-Strain Curves of Steel Alloys

**Ferrite**

**Ferrite + Martensite**
Micro-Structure & Plastic Deformation

- Ferrite
  - Plastic-Deformed Bainitic Ferrite
    - Austenite Film
    - Bainitic Ferrite Strengthening
- Bainite
- Martensite
  - Strain-Induced Martensite
  - Plastic-Deformed Martensite
- Austenite
  - Plastic-Deformed Austenite
  - Austenite Strengthening

The plastic-deformed phases
No deformed phases
Bainite Sub-Unit Size

Garcia-Mateo et al., 2011

1. Chemical Driving Force
2. Austenite Yield Strength
3. Temperature

\[ C_1 = \left( \sum x_n \omega_x \right) + \theta_1 \]

\[ H_1 = \tanh(C_1) \]
Mechanical Response of Bainite

Garcia-Mateo et al., 2011

Training

Prediction
Micro-Structure & Plastic Deformation

- Ferrite
  - Plastic-Deformed Bainitic Ferrite
    - Austenite Film
    - Bainitic Ferrite Strengthening
- Bainite
- Martensite
  - Strain-Induced Martensite
  - Plastic-Deformed Austenite
    - Austenite Strengthening
  - Plastic-Deformed Martensite

The plastic-deformed phases

No deformed phases
Parameters for Olson-Cohen Model

Olson et al., 1972, 1975


<table>
<thead>
<tr>
<th>Composition</th>
<th>O-C Param.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\alpha$, $\beta$</td>
</tr>
<tr>
<td>1 Fe-0.13C-1.42Mn-1.50Si</td>
<td>$\alpha=20$, $\beta=0.94$</td>
</tr>
<tr>
<td>2</td>
<td>$\alpha=26$, $\beta=0.94$</td>
</tr>
<tr>
<td>3</td>
<td>$\alpha=20$, $\beta=0.70$</td>
</tr>
<tr>
<td>4</td>
<td>-</td>
</tr>
<tr>
<td>5 Fe-0.16C-1.30Mn-0.38Si</td>
<td>$\alpha=57$, $\beta=1.41$</td>
</tr>
<tr>
<td>6</td>
<td>$\alpha=30$, $\beta=1.88$</td>
</tr>
<tr>
<td>7</td>
<td>$\alpha=49$, $\beta=2.08$</td>
</tr>
<tr>
<td>8</td>
<td>-</td>
</tr>
</tbody>
</table>

\[ Vf_{\alpha'} = 1 - \exp \left[ -\beta \left( 1 - \exp(-\alpha\varepsilon) \right)^n \right] \]

\[ \tau_{YS} = \tau_0 + \kappa D^{-\frac{1}{2}} \]
Parameters for Olson-Cohen Model

\[ V f_{\alpha'} = 1 - \exp \left[ -\beta \left( 1 - \exp(-\alpha \varepsilon) \right)^n \right] \]

Jacques et al., Philosophical Magazine A, 2001

Strain Rate = 2 mm/min = 6.67E-4 s\(^{-1}\)

<table>
<thead>
<tr>
<th>Composition</th>
<th>(T_{\text{BIT}}, \text{K})</th>
<th>(\Delta G, \text{J/mol})</th>
<th>O-C Param.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe-0.13C-1.42Mn-1.50Si</td>
<td>683</td>
<td>-1785</td>
<td>(\alpha=20, \beta=0.94)</td>
</tr>
<tr>
<td></td>
<td>633</td>
<td>-2239</td>
<td>(\alpha=26, \beta=0.94)</td>
</tr>
<tr>
<td></td>
<td>683</td>
<td>-1860</td>
<td>(\alpha=20, \beta=0.70)</td>
</tr>
<tr>
<td>Fe-0.16C-1.30Mn-0.38Si</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>643</td>
<td>-2216</td>
<td>(\alpha=57, \beta=1.41)</td>
</tr>
<tr>
<td></td>
<td>643</td>
<td>-2216</td>
<td>(\alpha=30, \beta=1.88)</td>
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<tr>
<td></td>
<td>643</td>
<td>-2216</td>
<td>-</td>
</tr>
</tbody>
</table>
The Optimum Conditions for TRIP Steels

1. Total alloying addition is less than 4 wt%.
2. 10 individuals in one generation, 1,000 generations.
3. Full equilibrium after IA treatment is considered.
4. $T_0$ and para $\gamma - \theta$ concepts are utilized.
Phase Constituent and Performance

Vf(Fer)

Vf(Mar)

Vf(Bai)

Vf(Aus)
Chemical Composition and Performance
To achieve 15%-1600MPa, the recommended conditions are (wt%; K):

<table>
<thead>
<tr>
<th></th>
<th>C</th>
<th>Mn</th>
<th>Si</th>
<th>$T_{IA}$</th>
<th>$T_{BIT}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0.24</td>
<td>0.48</td>
<td>2.22</td>
<td>1051</td>
<td>601</td>
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</tbody>
</table>
Conclusion

Composition Selection

C Mn Si Al

Genetic Algorithm

Mechanical Properties

Micro-Structure

Mechanical Model based on Irreversible Thermodynamics

CALPHAD Method
Selected References

1. S Li et al., Thermodynamic analysis of two-stage heat treatment in TRIP steels
2. S Li et al., Development of a Kinetic Model for Bainitic Isothermal Transformation in Transformation-Induced Plasticity Steels
4. Caballero et al., Design of Advanced Bainitic Steels by Optimisation of TTT Diagrams and T0 Curves
5. Xu et al., Genetic alloy design based on thermodynamics and kinetics
6. Matsumura et al., Mechanical properties and retained austenite in intercritically heat-treated bainite-transformed steel and their variation with Si and Mn additions
7. De Cooman, Structure–properties relationship in TRIP steels containing carbide-free bainite