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\textsuperscript{1} Tata Steel  
\textsuperscript{2} MPIE

\textbf{Predicting the $M_s$ temperature of steels with a thermodynamic based model including the effect of the prior austenite grain size}

28 June 2017  
GTT-Technologies meeting

* This work has been conducted in the framework of RFCS project ToolMart

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Outline

1. Introduction
2. Effect of Prior Austenite Grain Size on $M_s$ temperature
3. $T_1$ model to replace thermodynamic calculations
4. Validation of the new $M_s$ model
5. Benchmarking of the new $M_s$ model
Martensite

Adolf Martens
1850-1914
Martensite start ($M_s$) temperature versus Carbon content

Fig. 9. Martensite transformation start temperatures ($M_s$) vs carbon content. The range of compositions in which the various types of martensite exist is also shown.

Courtesy: Marder and Krauss (1967)
Effect of Austenite Grain Size on $M_s$

- **1a** Variation of $M_s$ with austenitizing temperature for an En23 steel

- **Sastri, 1965**

- **Yang, 2009**
Schematic of the modeling approach

A. Modeling the effect of $D_\gamma$ on $M_s$: adding the terms $W_{HP}$ and $W_C$ to the Ghosh model.

- $W_{HP}$: Hall-Petch strengthening of $\gamma$ grains
- $W_C$: to account for change in aspect ratio of laths below a critical $D_\gamma$

B. $T_1$ model derivation.

- Nearby $M_s$:
  - $\Delta G_c/dT = 7.22$ J/molK
  - $\Delta G_c = 7.22 \times (T_1 - M_s)$
  - $T_1 = f$ (composition)

C. Schematic of the new model to calculate $M_s$:

- $\Delta G_c = K_1 + W_\mu + W_{HP} + W_C$
- $M_s = T_1 - (\Delta G_c / 7.22)$
The definition of $T_0$

\[ \frac{\Delta G}{\Delta C} = 0 \]
Martensitic transformations require large undercooling below $T_0$

$M_s < T < T_0 \quad (\Delta G > 0, \text{ but } \Delta G < \Delta G_c)$
Definition of the critical driving force $\Delta G_c$

\[ T = M_s \quad (\Delta G = \Delta G_c) \]
Ghosh and Olson model (1994)

\[ \Delta G_c = K_1 + W_\mu (K_\mu^i, x_i) \]

\[ W_\mu = K_\mu x_C^{0.5} + \sqrt{\sum_j (K_j^i x_j^{0.5})^2} \]

- Modelling approach of Ghosh:
  - \( W_\mu \) : athermal interfacial frictional work
  - Specific superposition law (Phythagorean)
  - \( K_\mu \)'s found by model optimization

- This work:
  - \( j = \text{Mn, Si, Cr, Ni or Mo} \)

Modification/improvements:
- Account for Austenite Grain Size effects
- Validate model with \( M_s \) data of AHSS/UHSS grades
- Make model calculations without dependence on specific thermodynamic databases
Modified Ghosh model capturing $M_s$ dependence on $D^\gamma$

$$\Delta G_c = K_1 + W_\mu + W_{HP} + W_C$$

Austenite strengthening, Hall Petch mechanism (Ansell)
  - Higher YS of austenite $\rightarrow$ more resistance to shape deformation

$W_{HP} = \frac{K_{HP}}{\sqrt{D^\gamma}}$

Critical Austenite Grain Size, $D_c \sim 15$ micron (MPIE/AMMZ)
  - Change in aspect ratio laths $\rightarrow$ change in stored energy (Christian)

$W_C = K_C \exp\left( -\frac{6D^\gamma}{D_c} \right)$

(a) $W_{HP}$

$W_C$

$D_c = 15 \, \mu m$
Observations of lath aspect ratio (c/a)

Lutz Morsdorf: (MPIE)

- **Base alloy:** coarse grains
- **Base + Nb alloy:** small grains

- Length of packets is constrained by small PAGS.
- Lath thickness is ~200 nm for both alloys.
Ghosh model capturing $M_s$ dependence on $D^\gamma$

$$\Delta G_c = K_1 + W_\mu + W_{HP} + W_C$$

$$W_{HP} = \frac{K_{HP}}{\sqrt{D^\gamma}}$$

$$K_{HP} = 350 \text{ J} \mu\text{m}^{0.5}/\text{mol}$$

$$W_C = K_C \exp\left(-\frac{6D^\gamma}{D_C}\right)$$

$$K_C = 370 \text{ J/mol}$$

$$D_C = 15 \mu\text{m}$$

(b)

- $D^\gamma < D_C$: $W_C$ contribution
- $D^\gamma > D_C$: only $W_{HP}$ contribution
- Combined $W_{HP}$ and $W_C$
Validation of the model for $D^γ$ effect on $M_s$

\[ K_C = 370 \text{ J/mol}, \quad K_{HP} = 350 \mu \text{m}^{0.5}/\text{mol} \]

\[ D_C = 10 - 20 \mu \text{m} \text{ for most alloys} \]
Schematic of the modeling approach

A. Modeling the effect of $D^\gamma$ on $M_s$: adding the terms $W_{HP}$ and $W_C$ to the Ghosh model.

- $W_{HP}$: Hall-Petch strengthening of $\gamma$ grains
- $W_C$: to account for change in aspect ratio of laths below a critical $D^\gamma$

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- Nearby $M_s$:
  \[ \Delta G_c/dT = 7.22 \text{ J/molK} \]
  \[ \Delta G_c = 7.22 (T_1 - M_s) \]
  \[ T_1 = f(\text{composition}) \]

C. Schematic of the new model to calculate $M_s$:

- Composition
- $D^\gamma$
- $\Delta G_c = K_1 + W_\mu + W_{HP} + W_C$
- $M_s = T_1 - (\Delta G_c / 7.22)$
Calculations for Base alloy (0.22C-2.5Mn-0.2Cr-0.2Si)

Comparison of FactSage, MTData & JMatPro

\[ \Delta G \text{ [kJ/mol]} \]

- DG 0.22C (FactSage)
- DG 0.22C (JMatPro)
- DG 0.22C (MTData)

MTData: T0 = 651°C
FactSage: T0 = 652°C
JMatPro: T0 = 645°C
Calculations for Base alloy (0.22C-2.5Mn-0.2Si-0.2Cr)

### Graphical Data

**Relative differences in $\Delta G_c$ are a few percent**

- **DG 0.22C (FactSage)**
- **DG 0.22C (JMatPro)**
- **DG 0.22C (MTData)**

If $M_s = 365^\circ C$, then:
- $\Delta G = 1.63 \text{ kJ/mol (FactSage)}$
- $\Delta G = 1.62 \text{ kJ/mol (MTData)}$
- $\Delta G = 1.60 \text{ kJ/mol (JMatPro)}$

**Ms = 365^\circ C** (empirical prediction)

Relative differences in $\Delta G_c$ are a few percent.
Linear approximation of $\Delta G$ curves is valid nearby $M_s$

Calculations of $\Delta G$ were performed with FactSage

$\Delta G_c \approx 1740 \text{ J/mol}$

$M_s \approx 345 \text{ ºC}$

$T_0 = 627 \text{ ºC}$

$T_1 = 585 \text{ ºC}$

$\Delta G_c = 7.22 \left( T_1 - M_s \right)$

$T_1$ has no physical meaning, it is a mathematical parameter.
The linear dependence with slope of 7.22 J/molK seems valid for Fe-C alloys in general.

A rigorous investigation was started to

1. Confirm that linearity with a slope of 7.22 J/molK is applicable for all steels
2. Correlate $T_1$ temperatures to the chemical composition of steels
$T_1$ temperatures against C content

Determined with FactSage for plain carbon steels with 0.1Mn and 0.1Si

$$T_1 = 715 - 291 \degree C$$
**T₁ temperatures against C content**

Determined with FactSage for alloys with **2.0Mn, 0.2Si and 0.2Cr**

\[
T₁ = 668 - 291\text{C}
\]

- **T₁ dependency on Carbon is not affected by other alloying**
$T_1$ temperatures against Mn content

\[ T_1 = \text{Constant} - 24\text{Mn} \]

(a) Fe-0.47C-0.28Si + Mn
$T_1 = 581^\circ\text{C} - 24.2^\circ\text{C/wt% Mn}$

(b) Fe-0.22C-0.2Si-0.2Cr + Mn
$T_1 = 652^\circ\text{C} - 23.9^\circ\text{C/wt% Mn}$
$T_1$ temperatures against Si, Cr, Ni and Mo contents

Fe-0.47C-0.35Mn-0.28Si + X

Fe-0.22C-2.0Mn-0.2Si-0.2Cr + X

$T_1 = 718 - 291C - 24Mn - 1.5Si - 5.0Cr - 18.5Ni + 3.5Mo$
Validation $T_1$ equation with literature data

$$T_1 = 718.3 - 291x_C - 24x_{Mn} - 1.8x_{Si} - 5.6x_{Cr} - 18.4x_{Ni} + 3.5x_{Mo}$$

$T_1$ model benchmarked against FactSage results of $>$ 70 alloys:
- Largest deviations $\sim 3 \degree C$
- $\sigma \approx 1.2 \degree C$
Schematic of the modeling approach

A. Modeling the effect of $D^\gamma$ on $M_s$: adding the terms $W_{HP}$ and $W_C$ to the Ghosh model.

$W_{HP}$: Hall-Petch strengthening of $\gamma$ grains

$W_C$: to account for change in aspect ratio of laths below a critical $D^\gamma$

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Nearby $M_s$: $\Delta G_c/dT = 7.22$ J/molK

$\Delta G_c = 7.22 (T_1 - M_s)$

$T_1 = f$ (composition)

C. Schematic of the new model to calculate $M_s$:

- Composition
- $T_1$ model
- $\Delta G_c = K_1 + W_\mu + W_{HP} + W_C$

$M_s = T_1 - (\Delta G_c / 7.22)$
### Table 1. Data of alloys used for the validation of the models for $T_c$, $D^r$ (G) and $M_c$.

<table>
<thead>
<tr>
<th>No.</th>
<th>Ref.</th>
<th>grade</th>
<th>C wt%</th>
<th>Mn wt%</th>
<th>Si wt%</th>
<th>Cr wt%</th>
<th>Ni wt%</th>
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<th>$T_c$</th>
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### Table 2. Data of 62–121 alloys used for the validation of the $M_c$ model.

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### ToolMart (2016)

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<th>$D^r$</th>
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### Glanre (1946)

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### Steven (1956)

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### Payson (1944)

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### TTT diagrams

**ASM (1991)**

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### Rowland (1946)

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<td>1.00</td>
<td>590</td>
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</table>
Validation of the new $M_s$ model

$$
\Delta G_c = K_1 + W_\mu + \frac{K_{\text{HP}}}{\sqrt{D^\gamma}} + K_C \exp \left( - \frac{6D^\gamma}{D_C} \right)
$$

$K_1 = 1015 \, \text{J/mol}$ \hspace{1cm} $W_\mu = 670x_C^{0.5} + \sqrt{(195x_{Mn}^{0.5})^2 + (140x_{Si}^{0.5})^2 + (170x_{Cr}^{0.5})^2 + (5x_{Ni}^{0.5})^2 + (205x_{Mo}^{0.5})^2}$

$K_{\text{HP}} = 350 \, \mu\text{m}^{0.5/\text{mol}}$

$K_C = 370 \, \text{J/mol}$

$D_C = 11 \, \mu\text{m}$

Alloying ranges tested:
0.1 - 0.7 C
0 - 3 Mn
0 - 2 Si
0 - 3 Cr
0 - 5 Ni
0 - 1 Mo

Largest deviations $\approx 20 \degree C$

$\sigma \approx 7 \degree C$
## Benchmarking to other models

### Table: standard errors associated with different models tested against alloys 1-121

<table>
<thead>
<tr>
<th>Model</th>
<th>$\sigma$ (ºC)</th>
<th>$\sigma$ (ºC) evaluated for various datasets (alloy series)</th>
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<tbody>
<tr>
<td>Payson (1944)</td>
<td>$17$</td>
<td>37</td>
</tr>
<tr>
<td>Carapella (1944)</td>
<td>$23$</td>
<td>48</td>
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<td>Nehrenberg (1946)</td>
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<td>25</td>
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<tr>
<td>Grange (1946)</td>
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<td>Steven (1956)</td>
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**Overall model performance**

**alloys 90-115: Payson data**
Thank you for your attention!

Do you have any questions?