Calculation of ε martensite and stacking fault energies in austenitic Fe-Mn-C alloys

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Motivation

Strength/deformation strongly controlled by austenite stability:
TRIP, TWIP, MBIP are possible

http://www.metalformingmagazine.com (original from WorldAutoSteel)
Experimental determination of SFE

Thermodynamic calculation of SFE

The molar surface density of (111) planes

\[ SFE = 2\rho\Delta G_{\gamma \rightarrow \epsilon} + 2\sigma \]

The molar Gibbs energy of the transformation \( \gamma \rightarrow \epsilon \)

\[ \rho = \frac{4}{\sqrt{3}} \frac{1}{a^2N} \]

\[ A = \frac{\sqrt{3}}{4} a^2 \]

\[ \Delta G_{\gamma \rightarrow \epsilon} = G_{\epsilon}(hcp) - G_{\epsilon}(fcc) \]

Fe-Mn 25°C

Mass-% Mn

Gibbs energy, kJ/mol
Fe-Mn: Phase diagram


Fe-Mn: Gibbs energies

W. Huang, Calphad 13, 243 (1989).

Fe-Mn: Gibbs energy of hcp?

Driving force for $\varepsilon$ martensite formation: $\Delta G = 70$ J/mol

(This is the “distance” between $T_0$ and $M_s$)

Fe-Mn: $T_0$ for fcc/hcp and fcc/bcc

Driving force for $\varepsilon$ martensite formation: $\Delta G = 70 \text{ J/mol}$

(This is the “distance” between $T_0$ and $M_s$)

$\Delta G^{\gamma\rightarrow\alpha} = 1868 \text{ J/mol}$
Calculation of $T_0^{\gamma/\varepsilon}$ with Thermo-Calc

- Suspend all phases except fcc and hcp
- Calculate an equilibrium with fcc and hcp (e.g. $w$(Mn)=0.25, $T$=400)

- Single point:
  ADVANCED-OPTION T-ZERO FCC HCP

- Curve:
  SET-AXIS-VAR W(MN) 0 0.4 0.01
  STEP T-ZERO FCC HCP
Calculation of $M_s^{\gamma/\varepsilon}$ with Thermo-Calc

- Suspend all phases except fcc and hcp
- Shift the Gibbs energy of hcp by 70 J/mol
  ADV-OPT PHASE-ADDITION HCP 70
- Calculate an equilibrium with fcc and hcp (e.g. $w$(Mn)=0.25, $T$=400)
- Single point:
  ADVANCED-OPTION T-ZERO FCC HCP
- Curve:
  SET-AXIS-VAR W(MN) 0 0.4 0.01
  STEP T-ZERO FCC HCP
SFE in Fe-Mn

\[
SFE = 2\rho \Delta G^{\gamma\varepsilon} + 2\sigma
\]

\(\sigma = 15\)

\(\sigma = 5\)

Mass-% Mn
SFE in Fe-Mn?

The SFE in Fe-Mn is negative!
(for wt.% Mn < 27)


Volosevich (1974)
Schumann (1974)
Lee (2000); thermodyn. calc.

Fe-Mn-C: Driving force for ε-Martensite

Calculated γ/ε $T_0$ line

$\gamma / \varepsilon$ $T_0$ line


$(SFE = 2\rho \Delta G_{\gamma \rightarrow \varepsilon} + 2\sigma)$
Fe-Mn-C: ε-Martensite and SFE

The SFE increases by about 5 mJ/m² for each 0.1 wt.% C (assuming that σ is constant)

\[ SFE = 2\rho \Delta G^{\gamma \rightarrow \varepsilon} + 2\sigma \]
Fe-Mn-C: ε-Martensite and SFE

Calculated $\gamma/\varepsilon$ $T_0$ line

SFE as function of Mn content at 25 °C

$\sigma = 5 \text{ mJ/m}^2$

$SFE = 2\rho \Delta G^{\gamma \rightarrow \varepsilon} + 2\sigma$
Deformation mechanisms – $\Delta G^{\gamma \rightarrow \varepsilon}$

Thermodynamic based calculation from L. Mosecker, A. Saeed-Akbari, IEHK, RWTH Aachen, 2011
Deformation mechanisms

\[ \sigma = 5 \text{ mJ/m}^2 \]

\( SFE \) as function of Mn content at 25 °C

\[ (SFE = 2\rho \Delta G_{\gamma\rightarrow\varepsilon} + 2\sigma) \]


Thermo-Calc user meeting, Aachen, Sep. 11-12, 2014
Conclusions

• There is strong connection between ε-martensite formation, SFE and deformation mechanisms.
• Data on ε-martensite formation can be used to model the hcp phase. $T_0$, $M_s$ and SFE can then be calculated/estimated.
• SFE < 0 : ε-martensite can grow spontaneously. Below $M_s$ SFE is negative.
• TRIP takes place between $M_s$ and $T_0$. TWIP takes place above $T_0$.
• The magnetic transition in fcc ($T_N$) causes non-linear effects.
Thank you for your attention!
Calculating $T_0$ with PARROT

ENTER CONSTANT P0=101325
ENTER CONSTANT T0=1
ENTER CONSTANT WMN=0.1
ENTER CONSTANT FEL=1
ENTER CONSTANT EX2=0

IMPORT T0#1
IMPORT WMN#2
IMPORT EX2#4
IMPORT FEL#10

$HCP
CREATE-NEW 1,1
CHANGE-STATUS PHASE HCP=FIX 1
SET-CONDITION P=P0, T=T0, W(MN)=WMN
ENTER VARIABLE GMHCP=GM(HCP);
EVALUATE GMHCP
$
$FCC
CREATE-NEW 2,1
CHANGE-STATUS PHASE FCC=FIX 1
SET-CONDITION P=P0, T=T0, W(MN)=WMN
ENTER VARIABLE GMFCC=GM(FCC);
EVALUATE GMFCC
ENTER VARIABLE EX1=(GMFCC-GMHCP);
$EXP
EXPERIMENT EX1=EX2:FEL
SAVE
END

- Read data from a database as usual
- Go to PARROT
- Create a store file
  CREATE-NEW-STORE-FILE
- Compile the POP-file (shown left)
  COMPILE-EXPERIMENTS
- Define variables (to “optimize” temperature)
  SET-OPT-VAR 1 400
  SET-FIX-VAR 2 0.25
  SET-FIX-VAR 4 0 (set to 70 for $M_s$)
  SET-FIX-VAR 10 1
- Optimize (several times until the error sum is very small)
  OPTIMIZE-VARIABLES
- V1 is now $T_0$
  LIST-ALL-VARIABLES