A Thermodynamic Assessment of the Fe-Cr-Ni-C System

by M. Hillert and C. Qiu

Pages 2195 through 2197:

Table II should be updated as follows:

Table II. Summary of Thermodynamic Parameters Describing the Fe-Cr-Ni-C System in SI Units (J, mol, K)*

Liquid

One sublattice, site 1 constituents: C, Cr, Fe, Ni

$$^{\circ}G_{\text{C}}^{\text{liq}} = ^{\circ}G_{\text{C}}^{\text{gra}} + 117,369 - 24.63T$$

$$^{\circ}G_{\text{Cr}}^{\text{liq}} = ^{\circ}G_{\text{Cr}}^{\text{hbcc}} + 24,335.93 - 11.42T + 2.37615 \cdot 10^{-21} T^7 \quad 298.15 < T < 2180$$

$$= H^{\text{SER}} - 16,459 + 335.618T - 50T \ln T \quad 2180 < T < 6000$$

$$^{\circ}G_{\text{Fe}}^{\text{liq}} = ^{\circ}G_{\text{Fe}}^{\text{hbcc}} + 12,040.17 - 6.55843T - 3.6751551 \cdot 10^{-21} T^7 \quad 298.15 < T < 1811$$

$$= H^{\text{SER}} - 10,839.7 + 291.302T - 46T \ln T \quad 1811 < T < 6000$$

$$^{\circ}G_{\text{Ni}}^{\text{liq}} = ^{\circ}G_{\text{Ni}}^{\text{hfcc}} + 16,414.686 - 9.397T - 3.82318 \cdot 10^{-21} T^7 \quad 298.15 < T < 1728$$

$$= H^{\text{SER}} - 9549.775 + 268.598T - 43.1T \ln T \quad 1728 < T < 6000$$

$$^0L_{\text{C,Cr}}^{\text{liq}} = -90,526 - 25.9116T$$

$$^1L_{\text{C,Cr}}^{\text{liq}} = 80,000$$

$$^2L_{\text{C,Cr}}^{\text{liq}} = 80,000$$

$$^0L_{\text{C,Fe}}^{\text{liq}} = -124,320 + 28.5T$$

$$^1L_{\text{C,Fe}}^{\text{liq}} = 19,300$$

$$^2L_{\text{C,Fe}}^{\text{liq}} = 49,260 - 19T$$

$$^0L_{\text{C,Ni}}^{\text{liq}} = -110,160 + 34.6T$$

$$^0L_{\text{Cr,Fe}}^{\text{liq}} = -14,550 + 6.65T$$

$$^0L_{\text{Cr,Ni}}^{\text{liq}} = -1276 - 5.3873T$$

$$^1L_{\text{Cr,Ni}}^{\text{liq}} = 2699$$

$$^0L_{\text{Fe,Ni}}^{\text{liq}} = -18,378.86 + 6.03912T$$

$$^1L_{\text{Fe,Ni}}^{\text{liq}} = -9228.1 - 3.54642T$$

$$*^0L_{\text{C,Cr,Fe}}^{\text{liq}} = -530,395$$

$$*^1L_{\text{C,Cr,Fe}}^{\text{liq}} = 49,287$$

$$*^2L_{\text{C,Cr,Fe}}^{\text{liq}} = 43,461$$

$$^0L_{\text{C,Fe,Ni}}^{\text{liq}} = 122,200 - 58.8T$$

$$^1L_{\text{C,Fe,Ni}}^{\text{liq}} = 92,200 - 58.8T$$

$$^2L_{\text{C,Fe,Ni}}^{\text{liq}} = 152,200 - 58.8T$$

$$^0L_{\text{Cr,Fe,Ni}}^{\text{liq}} = 13,022$$

$$^1L_{\text{Cr,Fe,Ni}}^{\text{liq}} = 13,177$$

$$^2L_{\text{Cr,Fe,Ni}}^{\text{liq}} = 3313$$

Bcc

Two sublattices, sites 1:3 constituents: Cr, Fe, Ni:C, Va

$$^{\circ}G_{\text{Cr}}^{\text{hbcc}} - H^{\text{SER}} = -8851.93 + 157.48T - 26.908T \ln T + 0.00189435T^2$$

$$- 1.47721 \cdot 10^{-6} T^3 + 139,250T^{-1} \quad 298.15 < T < 2180$$

$$= -34,864 + 344.18T - 50T \ln T - 2.88526 \cdot 10^{32} T^{-9} \quad 2180 < T < 6000$$

$$^{\circ}G_{\text{Fe}}^{\text{hbcc}} - H^{\text{SER}} = +1224.83 + 124.134T - 23.5143T \ln T - 0.00439752T^2$$

$$- 5.89269 \cdot 10^{-8} T^3 + 77,358.5T^{-1} \quad 298.15 < T < 1811$$

$$= -25,384.451 + 299.31255T - 46T \ln T + 2.2960305 \cdot 10^{31} T^{-9} \quad 1811 < T < 6000$$

$$^{\circ}G_{\text{Ni}}^{\text{hbcc}} = ^{\circ}G_{\text{Ni}}^{\text{hfcc}} + 8715.084 - 3.556T$$

$$^{\circ}G_{\text{Cr:C}}^{\text{hbcc}} = ^{\circ}G_{\text{Cr}}^{\text{hbcc}} + 3^{\circ}G_{\text{C}}^{\text{gra}} + 416,000$$

$$^{\circ}G_{\text{Fe:C}}^{\text{hbcc}} = ^{\circ}G_{\text{Fe}}^{\text{hbcc}} + 3^{\circ}G_{\text{C}}^{\text{gra}} + 322,050 + 75.667T$$

$$^{\circ}G_{\text{Ni:C}}^{\text{hbcc}} = ^{\circ}G_{\text{Ni}}^{\text{hfcc}} + 3^{\circ}G_{\text{C}}^{\text{gra}} + 400,000 - 100T$$

$$^0L_{\text{Cr:C,Va}}^{\text{bcc}} = -190T$$

$$^0L_{\text{Fe:C,Va}}^{\text{bcc}} = -190T$$

$$^0L_{\text{Cr,Fe:Va}}^{\text{bcc}} = 20,500 - 9.68T$$

$$*^0L_{\text{Cr,Fe:C}}^{\text{bcc}} = -1,226,000 + 570T$$

Table II. Cont. Summary of Thermodynamic Parameters Describing the Fe-Cr-Ni-C System in SI Units (J, mol, K)*

$$\begin{aligned}
{}^0L_{Cr,Ni:Va}^{bcc} &= 21,310 - 13.6585T \\
{}^1L_{Cr,Ni:Va}^{bcc} &= 25,800 - 7.8927T \\
*{}^0L_{Cr,Ni:C}^{bcc} &= -1,226,000 + 570T \\
{}^0L_{Fe,Ni:Va}^{bcc} &= -956.63 - 1.28726T \\
{}^1L_{Fe,Ni:Va}^{bcc} &= 1789.03 - 1.92912T \\
{}^0L_{Fe,Ni:C}^{bcc} &= -956.63 - 1.28726T \\
{}^1L_{Fe,Ni:C}^{bcc} &= 1789.03 - 1.92912T \\
{}^0L_{Cr,Fe,Ni:Va}^{bcc} &= 1390 \\
G_m^{mo} &= RT \ln(\beta + 1)f(\tau) \quad \tau = T/T_C \\
f(\tau) &= \frac{1}{\tau A} \left[\tau A - \frac{79}{140p} - \frac{158}{497} \left(\frac{1}{p} - 1 \right) \left(\frac{\tau^4}{2} + \frac{\tau^{10}}{45} + \frac{\tau^{16}}{200} \right) \right] & \text{for } \tau < 1 \\
f(\tau) &= -\frac{1}{A} \left[\frac{\tau^{-5}}{10} + \frac{\tau^{-15}}{315} + \frac{\tau^{-25}}{1500} \right] & \text{for } \tau > 1 \\
\text{where } A &= \frac{518}{1125} \left[1 + \frac{790}{497} \left(\frac{1}{p} - 1 \right) \right] \\
p &= 0.4 \\
T_C &= -311.5(y_{Cr}y_{Va} + y_{Cr}y_C) + 1043(y_{Fe}y_{Va} + y_{Fe}y_C) + 575(y_{Ni}y_{Va} + y_{Ni}y_C) \\
&\quad + y_{Cr}y_{Fe}(y_C + y_{Va})[1650 + 550(y_{Cr} - y_{Fe})] + y_{Cr}y_{Ni}y_{Va}[2373 + 617(y_{Cr} - y_{Ni})] \\
\beta &= -0.008(y_{Cr}y_{Va} + y_{Cr}y_C) + 2.22(y_{Fe}y_{Va} + y_{Fe}y_C) + 0.85(y_{Ni}y_{Va} + y_{Ni}y_C) \\
&\quad - 0.85y_{Cr}y_{Fe}(y_C + y_{Va}) + 4y_{Cr}y_{Ni}y_{Va} \\
\end{aligned}$$

Whenever the calculated value of T_C or β is negative, it should be divided by -1 when inserted in G_m^{mo} and $f(\tau)$.

Fcc

Two sublattices, sites 1:1 constituents: Cr, Fe, Ni:C, Va

$$\begin{aligned}
{}^0G_{Cr}^{hfcc} &= {}^0G_{Cr}^{hbcc} + 7284 + 0.163T \\
{}^0G_{Fe:Va}^{hfcc} &= {}^0G_{Fe}^{hbcc} - 1462.4 + 8.282T - 1.157T \ln T + 6.4 \cdot 10^{-4} T^2 & 298.15 < T < 1811 \\
&= H^{SER} - 27,098.266 + 300.25256T - 46T \ln T + 2.78854 \cdot 10^{31} T^{-9} & 1811 < T < 6000 \\
{}^0G_{Ni}^{hfcc} &= H^{SER} - 5179.159 + 117.854T - 22.096T \ln T - 0.0048407T^2 & 298.15 < T < 1728 \\
&= H^{SER} - 27,840.655 + 279.135T - 43.1T \ln T + 1.12754 \cdot 10^{31} T^{-9} & 1728 < T < 6000 \\
{}^0G_{Cr:C}^{hfcc} &= {}^0G_{Cr}^{hbcc} + {}^0G_C^{gra} + 25,000 \\
{}^0G_{Fe:C}^{hfcc} &= {}^0G_{Fe}^{hbcc} + {}^0G_C^{gra} + 77,202 - 15.877T \\
{}^0G_{Ni:C}^{hfcc} &= {}^0G_{Ni}^{hbcc} + {}^0G_C^{gra} + 45,000 + 1.88T \\
{}^0L_{Cr:C,Va}^{fcc} &= -29,686 - 18T \\
{}^0L_{Fe:C,Va}^{fcc} &= -34,671 \\
{}^0L_{Cr,Fe:Va}^{fcc} &= 10,833 - 7.477T \\
{}^1L_{Cr,Fe:Va}^{fcc} &= 1410 \\
{}^0L_{Cr,Fe:C}^{fcc} &= -26,586 - 18T \\
{}^0L_{Cr,Ni:Va}^{fcc} &= 8347 - 12.1038T \\
{}^1L_{Cr,Ni:Va}^{fcc} &= 29,895 - 16.3838T \\
{}^0L_{Cr,Ni:C}^{fcc} &= -81,265 + 81.8T \\
{}^0L_{Fe,Ni:Va}^{fcc} &= -12,054.355 + 3.27413T \\
{}^1L_{Fe,Ni:Va}^{fcc} &= 11,082.1315 - 4.45077T \\
{}^2L_{Fe,Ni:Va}^{fcc} &= -725.805174 \\
{}^0L_{Fe,Ni:C}^{fcc} &= 49,074 - 7.32T \\
{}^1L_{Fe,Ni:C}^{fcc} &= -25,800 \\
{}^0L_{Cr,Fe,Ni:Va}^{fcc} &= 1618 \\
*{}^0L_{Cr,Fe,Ni:C}^{fcc} &= -8215 \\
p &= 0.28 \\
T_C &= -1109y_{Cr}y_{Va} - 201(y_{Fe}y_{Va} + y_{Fe}y_C) + 633(y_{Ni}y_{Va} + y_{Ni}y_C) \\
&\quad - 3605y_{Cr}y_{Ni}y_{Va} + y_{Fe}y_{Ni}y_{Va}[2133 - 682(y_{Fe} - y_{Ni})] \\
\beta &= -2.46y_{Cr}y_{Va} - 2.1(y_{Fe}y_{Va} + y_{Fe}y_C) + 0.52(y_{Ni}y_{Va} + y_{Ni}y_C) - 1.91y_{Cr}y_{Ni}y_{Va} \\
&\quad - y_{Fe}y_{Ni}y_{Va}[9.55 + 7.23(y_{Fe} - y_{Ni}) + 5.93(y_{Fe} - y_{Ni})^2 + 6.18(y_{Fe} - y_{Ni})^3] \\
\end{aligned}$$

Whenever the calculated value of T_C or β is negative, it should be divided by -3 when inserted in G_m^{mo} and $f(\tau)$.

Table II. Cont. Summary of Thermodynamic Parameters Describing the Fe-Cr-Ni-C System in SI Units (J, mol, K)*

Graphite

Constituent: C

$$^{\circ}G_{\text{C}}^{\text{gra}} - H^{\text{SER}} = -17,369 + 170.73T - 24.3T \ln T - 4.723 \cdot 10^{-4} T^2 + 2,562,600T^{-1} \\ - 2.643 \cdot 10^8 T^{-2} + 1.2 \cdot 10^{10} T^{-3}$$

Cementite

Two sublattices, sites 3:1 constituents: Cr, Fe, Ni:C

$$^{\circ}G_{\text{Cr:C}}^{\text{cem}} = 3^{\circ}G_{\text{Cr}}^{\text{hbcc}} + ^{\circ}G_{\text{C}}^{\text{gra}} - 29,392 + 41.65T - 9.32T \ln T + 2.6282 \cdot 10^{-3} T^2$$

$$^{\circ}G_{\text{Fe:C}}^{\text{cem}} - H^{\text{SER}} = -10,745 + 706.04T - 120.6T \ln T$$

$$^{\circ}G_{\text{Ni:C}}^{\text{cem}} - H^{\text{SER}} = 3^{\circ}G_{\text{Ni}}^{\text{hfcc}} + ^{\circ}G_{\text{C}}^{\text{gra}} + 34,700 - 20T$$

$$^{\circ}L_{\text{Cr,Fe:C}}^{\text{cem}} = 20,976 - 20.3144T$$

$$^{\circ}L_{\text{Fe,Ni:C}}^{\text{cem}} = 29,400$$

Cr₃C₂

Two sublattices, sites 3:2 constituents: Cr:C

$$^{\circ}G_{\text{Cr:C}}^{\text{Cr}_3\text{C}_2} - H^{\text{SER}} = -92,138 + 632.1755T - 105.6289T \ln T - 0.022348T^2$$

M₂₃C₆

Three sublattices, sites 20:3:6 constituents: Cr, Fe, Ni:Cr, Fe, Ni:C

$$^{\circ}G_{\text{Cr:Cr:Fe}}^{\text{M}_{23}\text{C}_6} - H^{\text{SER}} = -462,844 + 3200.2837T - 550.0669T \ln T - 0.2043663T^2$$

$$^{\circ}G_{\text{Cr:Fe:C}}^{\text{M}_{23}\text{C}_6} = 20/23^{\circ}G_{\text{Cr:Cr:C}}^{\text{M}_{23}\text{C}_6} + 3/23^{\circ}G_{\text{Fe:Fe:C}}^{\text{M}_{23}\text{C}_6}$$

$$^{\circ}G_{\text{Fe:Cr:C}}^{\text{M}_{23}\text{C}_6} = 20/23^{\circ}G_{\text{Fe:Fe:C}}^{\text{M}_{23}\text{C}_6} + 3/23^{\circ}G_{\text{Cr:Cr:C}}^{\text{M}_{23}\text{C}_6}$$

$$^{\circ}G_{\text{Fe:Fe:C}}^{\text{M}_{23}\text{C}_6} = 23/3^{\circ}G_{\text{Fe:C}}^{\text{cem}} - 5/3^{\circ}G_{\text{C}}^{\text{gra}} + 66,920 - 40T$$

$$^{\circ}G_{\text{Fe:Ni:C}}^{\text{M}_{23}\text{C}_6} = 20/23^{\circ}G_{\text{Fe:Fe:C}}^{\text{M}_{23}\text{C}_6} + 3/23^{\circ}G_{\text{Ni:Ni:C}}^{\text{M}_{23}\text{C}_6}$$

$$^{\circ}G_{\text{Ni:Fe:C}}^{\text{M}_{23}\text{C}_6} = 20/23^{\circ}G_{\text{Ni:Ni:C}}^{\text{M}_{23}\text{C}_6} + 3/23^{\circ}G_{\text{Fe:Fe:C}}^{\text{M}_{23}\text{C}_6}$$

$$^{\circ}G_{\text{Ni:Ni:C}}^{\text{M}_{23}\text{C}_6} = 23^{\circ}G_{\text{Ni}}^{\text{hfcc}} + 6^{\circ}G_{\text{C}}^{\text{gra}} + 212,988$$

$$^{\circ}G_{\text{Cr:Ni:C}}^{\text{M}_{23}\text{C}_6} = 20/23^{\circ}G_{\text{Cr:Cr:C}}^{\text{M}_{23}\text{C}_6} + 3/23^{\circ}G_{\text{Ni:Ni:C}}^{\text{M}_{23}\text{C}_6}$$

$$^{\circ}G_{\text{Ni:Cr:C}}^{\text{M}_{23}\text{C}_6} = 20/23^{\circ}G_{\text{Ni:Ni:C}}^{\text{M}_{23}\text{C}_6} + 3/23^{\circ}G_{\text{Cr:Cr:C}}^{\text{M}_{23}\text{C}_6}$$

$$^{\circ}L_{\text{Cr,Fe:Cr,Fe:C}}^{\text{M}_{23}\text{C}_6} = 604,852 - 158.6196T$$

$$^{\circ}L_{\text{Cr,Fe:Ni,Fe:C}}^{\text{M}_{23}\text{C}_6} = -1,914,930$$

$$^{\circ}L_{\text{Cr,Fe:Cr,Fe:C}}^{\text{M}_{23}\text{C}_6} = -1,914,930$$

M₇C₃

Two sublattices, sites 7:3 constituents: Cr, Fe, Ni:C

$$^{\circ}G_{\text{Cr:C}}^{\text{M}_7\text{C}_3} - H^{\text{SER}} = -177,506 + 1471.6421T - 249.2091T \ln T - 0.024006T^2$$

$$^{\circ}G_{\text{Fe:C}}^{\text{M}_7\text{C}_3} = 7^{\circ}G_{\text{Fe}}^{\text{hbcc}} + 3^{\circ}G_{\text{C}}^{\text{gra}} + 113,385 - 78.37T$$

$$^{\circ}G_{\text{Ni:C}}^{\text{M}_7\text{C}_3} = 7^{\circ}G_{\text{Ni}}^{\text{hfcc}} + 3^{\circ}G_{\text{C}}^{\text{gra}} + 193,000$$

$$^{\circ}L_{\text{Cr,Fe:C}}^{\text{M}_7\text{C}_3} = -131,281 + 53.4926T$$

$$^{\circ}L_{\text{Cr,Fe:Ni:C}}^{\text{M}_7\text{C}_3} = -41,451$$

$$^{\circ}L_{\text{Cr,Fe,Ni:C}}^{\text{M}_7\text{C}_3} = -323,854$$

Sigma

Three sublattices, sites 8:4:18 constituents: Fe, Ni:Cr:Cr, Fe, Ni

$$^{\circ}G_{\text{Fe:Cr:Cr}}^{\sigma} = 8^{\circ}G_{\text{Fe}}^{\text{hfcc}} + 22^{\circ}G_{\text{Cr}}^{\text{hbcc}} + 92,300 - 95.96T$$

$$^{\circ}G_{\text{Fe:Cr:Fe}}^{\sigma} = 8^{\circ}G_{\text{Fe}}^{\text{hfcc}} + 4^{\circ}G_{\text{Cr}}^{\text{hbcc}} + 18^{\circ}G_{\text{Fe}}^{\text{hbcc}} + 117,300 - 95.96T$$

$$^{\circ}G_{\text{Fe:Cr:Ni}}^{\sigma} = 8^{\circ}G_{\text{Fe}}^{\text{hfcc}} + 4^{\circ}G_{\text{Cr}}^{\text{hbcc}} + 18^{\circ}G_{\text{Ni}}^{\text{hbcc}}$$

$$^{\circ}G_{\text{Ni:Cr:Cr}}^{\sigma} = 8^{\circ}G_{\text{Ni}}^{\text{hfcc}} + 22^{\circ}G_{\text{Cr}}^{\text{hbcc}} + 173,460 - 188T$$

$$^{\circ}G_{\text{Ni:Cr:Fe}}^{\sigma} = 8^{\circ}G_{\text{Ni}}^{\text{hfcc}} + 4^{\circ}G_{\text{Cr}}^{\text{hbcc}} + 18^{\circ}G_{\text{Fe}}^{\text{hbcc}}$$

$$^{\circ}G_{\text{Ni:Cr:Ni}}^{\sigma} = 8^{\circ}G_{\text{Ni}}^{\text{hfcc}} + 4^{\circ}G_{\text{Cr}}^{\text{hbcc}} + 18^{\circ}G_{\text{Ni}}^{\text{hbcc}} + 175,400$$

*The parameters marked with * were assessed in the present work.

Correction to Metall. Trans. A, 1992, vol. 23A, pp. 135-48

The Effect of Ternary Trace Additions on the Nucleation and Growth of γ' Precipitates in an Al-4.2 At. Pct Ag Alloy
by N. Prabhu and J.M. Howe

Page 135:

In the first paragraph of the Introduction, the element Cd was mistakenly included with the element In in describing the effects of various trace elements on the nucleation rate of precipitates. The correct sentence (within the list) should have read:

(2) Trace elements can increase the nucleation rate
(a) by precipitating first and acting as heterogeneous nucleation sites for subsequent precipitates: *e.g.*, In has been shown to act as heterogeneous nuclei for the θ' and T_1 phases in Al-Cu and Al-Cu-Li alloys, respectively^[2] and (b) ...

Correction to Metall. Trans. A, 1992, vol. 23A, pp. 221-35

Influence of Long-Term Aging at 520 °C and 560 °C and the Superimposed Creep Stress on the Microstructure of 1.25Cr-0.5Mo Steel

by N. Gope, T. Mukherjee, and D.S. Sarma

Page 221:

The author footnote information for T. Mukherjee should read:

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