Effect of Solid Solution Elements on Solubility Products of Carbides and Nitrides in Ferrite: Thermodynamic Calculations

XUAN-WEI LEI, DA-YONG LI, XUE-HUI ZHANG, and TONG-XIANG LIANG

Thermodynamic calculation based on the two sublattice model are used to evaluate solubility products of titanium, niobium, vanadium carbide, and nitride in ferrite under the effect of solid solution alloy elements Mn and Ni, respectively. The results show that the calculated solubility products of these binary compounds in pure ferrite are closer to the solubility products by experimental measurements than the solubility products by thermodynamic calculations in previous studies. The solubility products in ferrite, on the condition that the total solid solution alloy content is relatively small, are given as follows:

$$\log^{\alpha} K_{\mathrm{TiC}} = 5.08 - \frac{11,048}{T} + 0.04[\text{wt pct Mn}] + \frac{62}{T}[\text{wt pct Ni}]$$

$$\log^{\alpha} K_{\mathrm{NbC}} = 5.72 - \frac{12,249}{T} + 0.06[\text{wt pct Mn}] + \frac{44}{T}[\text{wt pct Ni}]$$

$$\log^{\alpha} K_{\mathrm{VC}} = 6.02 - \frac{9563}{T} + \left(-0.04 + \frac{79}{T}\right)[\text{wt pct Mn}] + \left(-0.03 + \frac{80}{T}\right)[\text{wt pct Ni}]$$

$$\log^{\alpha} K_{\mathrm{TiN}} = 5.41 - \frac{16,997}{T} + 0.03[\text{wt pct Mn}] + \frac{32}{T}[\text{wt pct Ni}]$$

$$\log^{\alpha} K_{\mathrm{NbN}} = 5.51 - \frac{12,799}{T} + 0.05[\text{wt pct Mn}] + \frac{13}{T}[\text{wt pct Ni}]$$

$$\log^{\alpha} K_{\mathrm{VN}} = 4.94 - \frac{10,615}{T} + \left(-0.05 + \frac{85}{T}\right)[\text{wt pct Mn}] + \left(-0.03 + \frac{49}{T}\right)[\text{wt pct Ni}]$$

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I. INTRODUCTION

HEAT treatments, including annealing and tempering, are very effective and boastful techniques to improve the comprehensive mechanical properties of microalloyed steels. Besides microstructure, the formed precipitate in these processes is also one important component that affects its performance. The fraction of precipitates is a significant parameter in quantitatively analyzing the role of precipitates in improving mechanical properties. The deduced solubility product of carbide or nitride in pure ferrite by former researchers are commonly used to estimate its fraction.[1,2] A general consensus is that solubility products of carbide and nitride in pure ferrite are intensely small and solid solution alloy elements have a minor effect on the solubility products. Thus, even in a relatively high solid solution alloy steel, the solubility product of carbide or nitride in pure ferrite can be used to approximate the fraction of its precipitates.[3,4] However, the reasonableness of this approach has not been evaluated and systematic investigations on the effect of solid solution elements on solubility products of carbides and nitrides in ferrite have not been carried out. In addition, nearly no exact solubility product expressions of carbide and nitride in ferrite containing solid solution elements have been reported in references.

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In this article, thermodynamic calculations are adopted to develop solubility products of titanium, niobium, vanadium carbide, and nitride in pure ferrite and to evaluate the effect of solid solution elements on solubility products of these carbides and nitrides. The calculation results are compared with previous studies to show their reliability. Thus, a reference of solubility products of these carbides and nitrides in ferrite containing solid solution elements can be obtained from this work.

II. THERMODYNAMIC CALCULATIONS TO EVALUATE SOLUBILITY PRODUCT OF FCC BINARY COMPOUND IN FERRITE

Consider the Fe-X_1-X_2-…-M-N system consisting of two components: α-Fe based solid solution (ferrite) and fcc structure compound. Thermodynamic calculations are based on several assumptions:

1. Both Gibbs energies of ferrite and compound can be described by the two-sublattice model. Fe, X_i, and M atoms fill in the first sublattice, and N atoms and Va fill in the second sublattice. Both the components can be described by the formula $(\mathrm{Fe}, X_1, X_2, \ldots, M)_a(N, \mathrm{Va})_b$; for ferrite, $a = 1$, $b = 3$, and for fcc phase, $a = 1$, $b = 1$.
2. The total content of solid solution elements in ferrite is relatively small. M and N elements are dilute in ferrite. Fe, X_i elements, and Va are dilute in the compound (the compound is approximately a binary compound).
3. Most of the Gibbs energies and interaction parameters L^{bcc} are diverse in the same order of magnitude or differ in one order of magnitude.
4. The equilibrium between the compound and ferrite is represented by the condition $\mu^{\mathrm{fcc}}_{M:N} = \mu^{\mathrm{bcc}}_{M} + \mu^{\mathrm{bcc}}_{N}$.

Based on assumption [1], the Gibbs energy of ferrite can be calculated as[7,8]

$$\begin{aligned} G^{\alpha} = & \sum y_j^{\alpha} \sum y_k^{\alpha\circ} G^{\mathrm{bcc}}_{j:k} + RT \sum y_j^{\alpha} \ln y_j^{\alpha} \\ & + 3RT \sum y_k^{\alpha} \ln y_k^{\alpha} \\ & + \sum y_j^{\alpha} \sum y_k^{\alpha} \left\{ \sum_{j'} y_{j'}^{\alpha} L^{\mathrm{bcc}}_{j,j':k} + \sum_{k'} y_{k'}^{\alpha} L^{\mathrm{bcc}}_{j:k,k'} \right\} + \ldots \\ & + {}^{mg}G^{\alpha} \end{aligned} \quad [1]$$

The expressions of ${}^{mg}G^{\alpha}$ are given as[9,10]

$${}^{mg}G^{\alpha} = RT \ln(\beta^{\mathrm{bcc}} + 1) f(\tau), \tau = T/T^{\mathrm{bcc}}_{\mathrm{c}} \quad [2a]$$

$$\begin{cases} \tau < 1, f(\tau) = 1 - \left[\dfrac{79\tau^{-1}}{140p} + \dfrac{474}{497}\dfrac{p-1}{p} \left(\dfrac{\tau^3}{6} + \dfrac{\tau^9}{135} + \dfrac{\tau^{15}}{600} \right) \right] \Big/ \left[\dfrac{518}{1125} + \dfrac{11,692}{15,975}\dfrac{1-p}{p} \right] \\ \tau > 1, f(\tau) = -\left(\dfrac{\tau^{-5}}{10} + \dfrac{\tau^{-15}}{315} + \dfrac{\tau^{-25}}{1500} \right) \Big/ \left[\dfrac{518}{1125} + \dfrac{11,692}{15,975}\dfrac{1-p}{p} \right] \end{cases} \quad [2b]$$

$$T^{\mathrm{bcc}}_{c} = \sum y_j^{\alpha 0} T^{\mathrm{bcc}}_{cj} + \sum_j y_j^{\alpha} \sum_{j'} y_{j'}^{\alpha} \sum_n {}^{n} T^{\mathrm{bcc}}_{cj,j'} \left(y_j^{\alpha} - y_{j'}^{\alpha} \right)^n \quad [2c]$$

$$\beta^{\mathrm{bcc}} = \sum y_j^{\alpha 0} \beta^{\mathrm{bcc}}_{j} + \sum_j y_j^{\alpha} \sum_{j'} y_{j'}^{\alpha} \sum_n {}^{n} \beta^{\mathrm{bcc}}_{j,j'} \left(y_j^{\alpha} - y_{j'}^{\alpha} \right)^n \quad [2d]$$

The following chemical potentials in ferrite can be calculated as

$$\begin{aligned} \mu^{\mathrm{bcc}}_{M} = \mu^{\mathrm{bcc}}_{M:\mathrm{Va}} = & G^{\alpha} + \frac{\partial G^{\alpha}}{\partial y^{\alpha}_{M}} + \frac{\partial G^{\alpha}}{\partial y^{\alpha}_{\mathrm{Va}}} \\ & - \left(y^{\alpha}_{\mathrm{Fe}} \frac{\partial G^{\alpha}}{\partial y^{\alpha}_{\mathrm{Fe}}} + \sum_i y^{\alpha}_{X_i} \frac{\partial G^{\alpha}}{\partial y^{\alpha}_{X_i}} + y^{\alpha}_{M} \frac{\partial G^{\alpha}}{\partial y^{\alpha}_{M}} + y^{\alpha}_{N} \frac{\partial G^{\alpha}}{\partial y^{\alpha}_{N}} + y^{\alpha}_{\mathrm{Va}} \frac{\partial G^{\alpha}}{\partial y^{\alpha}_{\mathrm{Va}}} \right) \end{aligned} \quad [3a]$$

$$\begin{aligned} \mu^{\mathrm{bcc}}_{M:N} = & G^{\alpha} + \frac{\partial G^{\alpha}}{\partial y^{\alpha}_{M}} + \frac{\partial G^{\alpha}}{y^{\alpha}_{N}} \\ & - \left(y^{\alpha}_{\mathrm{Fe}} \frac{\partial G^{\alpha}}{\partial y^{\alpha}_{\mathrm{Fe}}} + \sum_i y^{\alpha}_{X_i} \frac{\partial G^{\alpha}}{\partial y^{\alpha}_{X_i}} + y^{\alpha}_{M} \frac{\partial G^{\alpha}}{\partial y^{\alpha}_{M}} + y^{\alpha}_{N} \frac{\partial G^{\alpha}}{\partial y^{\alpha}_{N}} + y^{\alpha}_{\mathrm{Va}} \frac{\partial G^{\alpha}}{\partial y^{\alpha}_{\mathrm{Va}}} \right) \end{aligned} \quad [3b]$$

$$\mu^{\mathrm{bcc}}_{N} = \frac{1}{3} \left(\mu^{\mathrm{bcc}}_{M:N} - \mu^{\mathrm{bcc}}_{M:\mathrm{Va}} \right) = \frac{1}{3} \left(\frac{\partial G^{\alpha}}{y^{\alpha}_{N}} - \frac{\partial G^{\alpha}}{\partial y^{\alpha}_{\mathrm{Va}}} \right) \quad [3c]$$

The exact expressions of $\frac{\partial G^{\alpha}}{\partial y^{\alpha}_{\mathrm{Fe}}}$, $\frac{\partial G^{\alpha}}{\partial y^{\alpha}_{X_i}}$, $\frac{\partial G^{\alpha}}{\partial y^{\alpha}_{M}}$, $\frac{\partial G^{\alpha}}{\partial y^{\alpha}_{N}}$, and $\frac{\partial G^{\alpha}}{\partial y^{\alpha}_{\mathrm{Va}}}$ are given in the "Appendix". The approximate relationships between site fractions in the preceding thermodynamic equations and mole fractions in the system are established based on assumption [2] as

$$y^{\alpha}_{\mathrm{Fe}} = x_{\mathrm{Fe}}/(1 - x_N) \cong x_{\mathrm{Fe}} \quad [4a]$$

$$y^{\alpha}_{X_i} = x_{X_i}/(1 - x_N) \cong x_{X_i} \quad [4b]$$

$$y^{\alpha}_{M} = x_{M}/(1 - x_N) \cong x_{M} \quad [4c]$$

$$y^{\alpha}_{N} = \frac{1}{3} x_N \quad [4d]$$

$$y^{\alpha}_{\mathrm{Va}} = 1 - y^{\alpha}_{N} \cong 1 \quad [4e]$$

$$x_{\mathrm{Fe}} + \sum_i x_{X_i} \cong y^{\alpha}_{\mathrm{Fe}} + \sum_i y^{\alpha}_{X_i} = 1 - y^{\alpha}_{M} \cong 1 \quad [4f]$$

Replace y^{α}_{Fe}, $y^{\alpha}_{X_i}$, y^{α}_{M}, y^{α}_{N}, and y^{α}_{Va} in the expressions of $\frac{\partial G^{\alpha}}{\partial y^{\alpha}_{\mathrm{Fe}}}$, $\frac{\partial G^{\alpha}}{\partial y^{\alpha}_{X_i}}$, $\frac{\partial G^{\alpha}}{\partial y^{\alpha}_{M}}$, $\frac{\partial G^{\alpha}}{\partial y^{\alpha}_{N}}$, and $\frac{\partial G^{\alpha}}{\partial y^{\alpha}_{\mathrm{Va}}}$ with x_{Fe}, x_{X_i}, x_M, $\frac{1}{3}x_N$, and 1, respectively. Based on assumptions [2] and [3], the terms containing factor x_M, x_N, or $x_{X_i} x_{X_{i'}}$, which are actually

small terms in these expressions, can be ignored. Substituting these expressions into Eqs. [3a] and [3c] gives

$$\mu_M^{\text{bcc}} \cong {}^{\circ}G_{M:\text{Va}}^{\text{bcc}} + \text{R}T\ln x_M + x_{\text{Fe}}L_{\text{Fe},M:\text{Va}}^{\text{bcc}} + \sum_i x_{X_i}L_{X_i,M:\text{Va}}^{\text{bcc}} - \sum_i x_{\text{Fe}}x_{X_i}L_{\text{Fe},X_i:\text{Va}}^{\text{bcc}} + {}^{mg}\mu_M^{\text{bcc}}(x_{\text{Fe}}, x_{X_1}, x_{X_2}, \ldots) \quad [5a]$$

$$\begin{aligned}{}^{mg}\mu_M^{\text{bcc}}(x_{\text{Fe}}, x_{X_1}, x_{X_2}, \cdots) &= RTf(\tau)\ln\left(\beta^{\text{bcc}}+1\right) \\ &+ RT\tau\frac{\text{d}f(\tau)}{\text{d}\tau}\ln\left(\beta^{\text{bcc}}+1\right) - RTf(\tau) \\ &- RT\frac{\text{d}f(\tau)}{\text{d}\tau}\frac{\tau}{T_c^{\text{bcc}}}\left[{}^0T_{cM}^{\text{bcc}} + x_{\text{Fe}}\sum_n {}^nT_{c\text{Fe},M}^{\text{bcc}}\left(x_{\text{Fe}}-y_M^{\alpha}\right)^n \right. \\ &+ \sum_i x_{X_i}\sum_n {}^nT_{cX_i,M}^{\text{bcc}}\left(y_{X_i}^{\alpha}-y_M^{\alpha}\right)^n \\ &- \sum_i x_{\text{Fe}}x_{X_i}\sum_n n^nT_{c\text{Fe},X_i}^{\text{bcc}}x_{\text{Fe}}\left(x_{\text{Fe}}-y_{X_i}^{\alpha}\right)^{n-1} \\ &\left. - \sum_i x_{\text{Fe}}x_{X_i}\sum_n {}^nT_{c\text{Fe},X_i}^{\text{bcc}}\left(y_{\text{Fe}}^{\alpha}-y_{X_i}^{\alpha}\right)^n\right]\ln\left(\beta^{\text{bcc}}+1\right) \\ &+ RTf(\tau)\frac{1}{\beta^{\text{bcc}}+1}\left[{}^0\beta_M^{\text{bcc}} + x_{\text{Fe}}\sum_n {}^n\beta_{\text{Fe},M}^{\text{bcc}}\left(y_{\text{Fe}}^{\alpha}-y_M^{\alpha}\right)^n \right. \\ &+ \sum_i x_{X_i}\sum_n {}^n\beta_{X_i,M}^{\text{bcc}}\left(y_{X_i}^{\alpha}-y_M^{\alpha}\right)^n + 1 \\ &- \sum_i x_{\text{Fe}}x_{X_i}\sum_n n^n\beta_{\text{Fe},X_i}^{\text{bcc}}x_{\text{Fe}}\left(x_{\text{Fe}}-y_{X_i}^{\alpha}\right)^{n-1} \\ &\left. - \sum_i x_{\text{Fe}}x_{X_i}\sum_n {}^n\beta_{\text{Fe},X_i}^{\text{bcc}}\left(y_{\text{Fe}}^{\alpha}-y_{X_i}^{\alpha}\right)^n\right] \end{aligned} \quad [5b]$$

$$\begin{aligned}\mu_N^{\text{bcc}} &\cong x_{\text{Fe}}\left({}^{\circ}G_{\text{Fe}:N}^{\text{bcc}} - {}^{\circ}G_{\text{Fe}:\text{Va}}^{\text{bcc}}\right)\Big/3 \\ &+ \sum_i x_{X_i}\left({}^{\circ}G_{X_i:N}^{\text{bcc}} - {}^{\circ}G_{X_i:\text{Va}}^{\text{bcc}}\right)\Big/3 \\ &+ \text{R}T\ln x_N - \text{R}T\ln 3 + \left(x_{\text{Fe}}L_{\text{Fe}:N,\text{Va}}^{\text{bcc}} + \sum_i x_{X_i}L_{X_i:N,\text{Va}}^{\text{bcc}}\right)\Big/3 \\ &+ \sum_i x_{\text{Fe}}x_{X_i}\left(L_{\text{Fe},X_i:N}^{\text{bcc}} - L_{\text{Fe},X_i:\text{Va}}^{\text{bcc}}\right)\Big/3\end{aligned} \quad [5c]$$

Without considering the magnetic contribution to Gibbs energy of the compound, the following chemical potential can be calculated based on assumptions [1] through [3] in the same way:

$$\mu_{M:N}^{\text{fcc}} \cong {}^{\circ}G_{M:N}^{\text{fcc}} \quad [6]$$

Therefore, based on assumption [4], the following equations are established:

$$\text{R}T\ln x_Mx_N \cong \Delta G_{MN}^{\alpha}(x_{\text{Fe}}, x_{X_1}, x_{X_2}, \cdots) - {}^{mg}\mu_M^{\text{bcc}}(x_{\text{Fe}}, x_{X_1}, x_{X_2}, \cdots) + \text{R}T\ln 3 \quad [7a]$$

$$\begin{aligned}\Delta G_{MN}^{\alpha}(x_{\text{Fe}}, x_{X_1}, x_{X_2}, \cdots) &= \left({}^{\circ}G_{M:N}^{\text{fcc}} - {}^{\circ}G_{M:\text{Va}}^{\text{bcc}}\right) \\ &- x_{\text{Fe}}\left({}^{\circ}G_{\text{Fe}:N}^{\text{bcc}} - {}^{\circ}G_{\text{Fe}:\text{Va}}^{\text{bcc}}\right)\Big/3 - \sum_i x_{X_i}\left({}^{\circ}G_{X_i:N}^{\text{bcc}} - {}^{\circ}G_{X_i:\text{Va}}^{\text{bcc}}\right)\Big/3 \\ &- x_{\text{Fe}}L_{\text{Fe},M:\text{Va}}^{\text{bcc}} - \sum_i x_{X_i}L_{X_i,M:\text{Va}}^{\text{bcc}} + \sum_i x_{\text{Fe}}x_{X_i}L_{\text{Fe},X_i:\text{Va}}^{\text{bcc}} \\ &- \left(x_{\text{Fe}}L_{\text{Fe}:N,\text{Va}}^{\text{bcc}} + \sum_i x_{X_i}L_{X_i:N,\text{Va}}^{\text{bcc}}\right)\Big/3 \\ &- \sum_i x_{\text{Fe}}x_{X_i}\left(L_{\text{Fe},X_i:N}^{\text{bcc}} - L_{\text{Fe},X_i:\text{Va}}^{\text{bcc}}\right)\Big/3\end{aligned} \quad [7b]$$

Atomic fraction can be converted to weight percentage as

$$x_M \cong \frac{1}{100}[\text{wt pct } M]\frac{A_{\text{Fe}}\left(1-\sum_i x_{X_i}\right)+\sum_i x_{X_i}A_{X_i}}{A_M} \quad [8a]$$

$$x_N \cong \frac{1}{100}[\text{wt pct } N]\frac{A_{\text{Fe}}\left(1-\sum_i x_{X_i}\right)+\sum_i x_{X_i}A_{X_i}}{A_N} \quad [8b]$$

The logarithmic solubility product of fcc binary compound MN in ferrite is thus expressed as

$$\begin{aligned}\log^{\alpha}K_{MN} &= \log[\text{wt pct } M][\text{wt pct } N] \\ &\cong \frac{\left[\Delta G_{MN}^{\alpha}(x_{\text{Fe}}, x_{X_1}, x_{X_2}, \cdots) - {}^{mg}\mu_M^{\text{bcc}}(x_{\text{Fe}}, x_{X_1}, x_{X_2}, \cdots)\right]}{RT}\ln 10 \\ &- \log\frac{\left[A_{\text{Fe}}\left(1-\sum_i x_{X_i}\right)+\sum_i x_{X_i}A_{X_i}\right]^2}{A_MA_N} + 4 + \log 3\end{aligned} \quad [9]$$

When $\sum_i x_{X_i} = 0$, the logarithmic solubility product of fcc binary compound MN in pure ferrite is given as

$$\log {}^{\alpha}K_{MN}^0 \cong \left[\Delta G_{MN}^{\alpha}(1,0,0,\ldots) - {}^{mg}\mu_M^{\text{bcc}}(1,0,0,\ldots)\right]\Big/ RT\ln 10 - \log\frac{A_{\text{Fe}}^2}{A_MA_N} + 4 + \log 3 \quad [10]$$

When $i = 1$, the logarithmic solubility product of fcc binary compound MN in ferrite is given as

$$\log {}^{\alpha}K_{MN}^{X_1} \cong \left[\Delta G_{MN}^{\alpha}(x_{\text{Fe}}, x_{X_1}, 0, \ldots) - {}^{mg}\mu_M^{\text{bcc}}(x_{\text{Fe}}, x_{X_1}, 0, \ldots)\right]\Big/ RT\ln 10 - \log\frac{\left[A_{\text{Fe}}(1-x_{X_1})+x_{X_1}A_{X_1}\right]^2}{A_MA_N} + 4 + \log 3 \quad [11]$$

Thus, the increment of the logarithmic solubility product of fcc binary compound MN in ferrite for solid solution element X_1 addition is calculated as

$$\Delta\log\ {}^{\alpha}K_{MN}^{X_1} = \log{}^{\alpha}K_{MN}^{X_1} - \log{}^{\alpha}K_{MN}^{0} \quad [12]$$

The following relationship is given (the derivation process is seen in the "Appendix)":

$$\log\ {}^{\alpha}K_{MN} \cong \log\ {}^{\alpha}K_{MN}^{0} + \Delta\log\ {}^{\alpha}K_{MN}^{X_1} + \Delta\log\ {}^{\alpha}K_{MN}^{X_2} + \ldots \quad [13]$$

III. RESULTS

A. *Solubility Products of Carbide and Nitride in Pure Ferrite*

The general form of solubility product is expressed as

$$\log K_{MN} = A - B/T \quad [14]$$

where A and B are constants and T is the temperature in Kelvin. In the Fe-M-N system, when M is considered Ti, Nb, or V and N, C, or N, the solubility products of TiC, NbC, VC, TiN, NbN, and VN in pure ferrite can be calculated, respectively, inserting the thermodynamic parameters given in Tables AI through AIII into Eq. [9]. The calculated solubility products of carbides and nitrides in pure ferrite in the temperature range of 750 K to 1000 K are shown in Figure 1. It can be seen that the results match the general consensus that solubility products of carbide and nitride in pure ferrite are intensely small. The points in Figure 1 are fitted with Eq. [14]. The fitted results are shown in Figure 1 and Eqs. [15a] through [15f].

$$\log^{\alpha}K_{\mathrm{TiC}}^{0} = 5.08 - \frac{11,048}{T} \quad [15a]$$

$$\log^{\alpha}K_{\mathrm{NbC}}^{0} = 5.72 - \frac{12,249}{T} \quad [15b]$$

$$\log^{\alpha}K_{\mathrm{VC}}^{0} = 6.02 - \frac{9563}{T} \quad [15c]$$

$$\log^{\alpha}K_{\mathrm{TiN}}^{0} = 5.41 - \frac{16,997}{T} \quad [15d]$$

$$\log^{\alpha}K_{\mathrm{NbN}}^{0} = 5.51 - \frac{12,799}{T} \quad [15e]$$

$$\log^{\alpha}K_{\mathrm{VN}}^{0} = 4.94 - \frac{10,615}{T} \quad [15f]$$

B. *Effect of Solid Solution Elements on Solubility Products of Carbide and Nitride in Ferrite*

Consider X_1 is Mn or Ni, M is Ti, Nb, or V, and N, C, or N. In the Fe-X_1-M-N system, with x_{X_1} given, $\Delta\log\ {}^{\alpha}K_{MN}^{\mathrm{Mn}}$ and $\Delta\log\ {}^{\alpha}K_{MN}^{\mathrm{Ni}}$ values of TiC, NbC, VC, TiN, NbN, and VN in ferrite are calculated by Eqs. [11] and [12]. Parameters in these two equations are seen in Tables AI through AIII. The calculation results are shown in Figures 2 and 3, respectively. They indicate

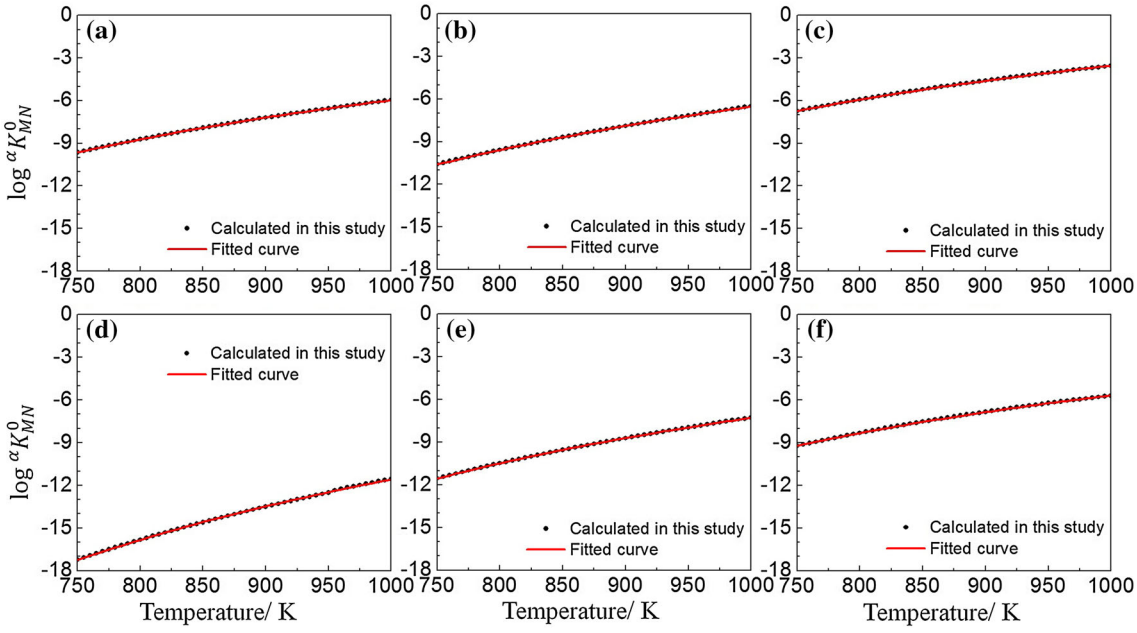

Fig. 1—Solubility products of carbides and nitrides in pure ferrite in this study: (*a*) TiC, (*b*) NbC, (*c*) VC, (*d*) TiN, (*e*) NbN, and (*f*) VN.

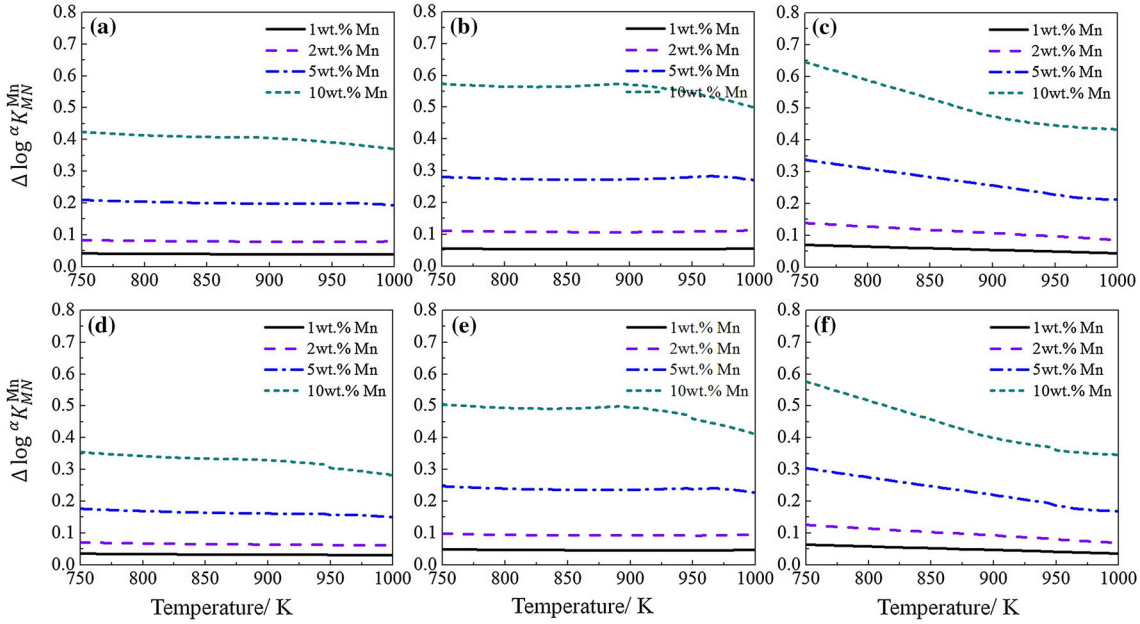

Fig. 2—Effect of different wt pct solid solution element Mn on solubility products of carbides and nitrides in ferrite in the Fe-Mn-*M*-*N* system in this study: (*a*) TiC, (*b*) NbC, (*c*) VC, (*d*) TiN, (*e*) NbN, and (*f*) VN.

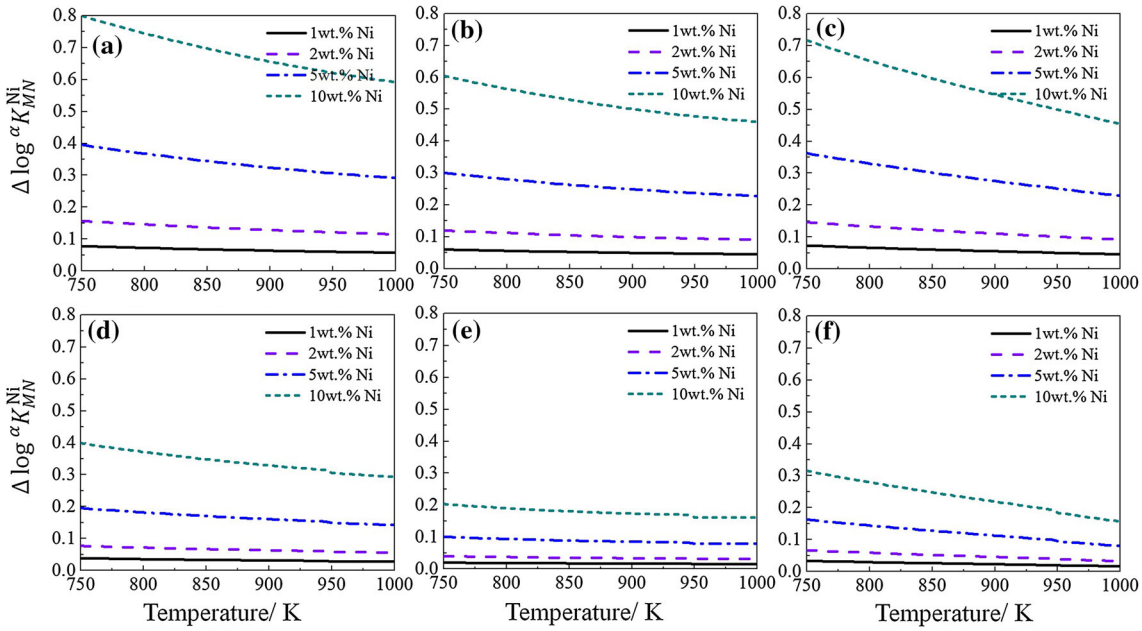

Fig. 3—Effect of different wt pct solid solution element Ni on solubility products of carbides and nitrides in ferrite in the Fe-Ni-*M*-*N* system in this study: (*a*) TiC, (*b*) NbC, (*c*) VC, (*d*) TiN, (*e*) NbN, and (*f*) VN.

that the solid solution element Mn or Ni in ferrite would increase the solubility products of these carbides and nitrides, but the increments are small and probably less than about 0.8 orders of magnitude even when the content of Mn or Ni is 10 wt pct. $\Delta\log\,{}^{\alpha}K_{MN}^{Mn}$ and $\Delta\log\,{}^{\alpha}K_{MN}^{Ni}$ are fitted with Eq. [14], respectively. Thus, the effect of solid solution elements on these solubility products in ferrite in the Fe-Mn-Ni-*M*-*N* system can be approximated as

$$\log^{\alpha} K_{\mathrm{TiC}} - \log\,{}^{\alpha}K^{0}_{\mathrm{TiC}} \cong 0.04[\text{wt pct Mn}] + \frac{62}{T}[\text{wt pct Ni}] \qquad [16a]$$

$$\log^{\alpha} K_{\mathrm{NbC}} - \log\,{}^{\alpha}K^{0}_{\mathrm{NbC}} \cong 0.06[\text{wt pct Mn}] + \frac{44}{T}[\text{wt pct Ni}] \qquad [16b]$$

Table I. Solubility Products of Carbides and Nitrides in Ferrite in Previous Studies

Compound	Solubility Products	Ref.	Description
TiC	$4.40 - 9575/T$	26	thermodynamic calculations
	$6.00 - 12,083/T$	27	thermodynamic calculations
	$5.02 - 10,800/T$	28	thermodynamic calculations
NbC	$3.90 - 9930/T$	26	thermodynamic calculations
	$3.46 - 8970/T$	28	thermodynamic calculations
	$5.43 - 10,960/T$	29	thermodynamic calculations
	$6.02 - 13,161/T$	30	thermodynamic calculations
VC	$4.55 - 8300/T$	31	best fit of the published solubility product data in temperature range 888 K to 1013 K
	$8.05 - 12,265/T$	26	thermodynamic calculations
	$2.72 - 6080/T$	32	experiment measurements in temperature range of 973 K to 1073 K
TiN	$5.89 - 16,750/T$	28	thermodynamic calculations
	$5.56 - 17,205/T$	33	extrapolation from solubility products in delta iron by thermodynamic calculations based on experiment measurements in temperature range of 1693 K to 1783 K
	$4.65 - 16,310/T$	34	thermodynamic calculations
NbN	$5.85 - 13,000/T$	28	thermodynamic calculations
	$4.96 - 12,230/T$	29	thermodynamic calculations
	$4.77 - 13,116/T$	35	thermodynamic calculations
VN	$0.12 - 5220/T$	32	experiment measurements in temperature range of 973 K to 1073 K
	$6.63 - 12,500/T$	36	thermodynamic calculations
	$2.45 - 7830/T$	37	thermodynamic calculations

$$\log^{\alpha} K_{\mathrm{VC}} - \log {}^{\alpha}K^{0}_{\mathrm{VC}} \cong \left(-0.04 + \frac{79}{T}\right)[\text{wt pct Mn}] + \left(-0.03 + \frac{80}{T}\right)[\text{wt pct Ni}] \quad [16c]$$

$$\log^{\alpha} K_{\mathrm{TiN}} - \log {}^{\alpha}K^{0}_{\mathrm{TiN}} \cong 0.03[\text{wt pct Mn}] + \frac{32}{T}[\text{wt pct Ni}] \quad [16d]$$

$$\log^{\alpha} K_{\mathrm{NbN}} - \log^{\alpha}K^{0}_{\mathrm{NbN}} \cong 0.05[\text{wt pct Mn}] + \frac{13}{T}[\text{wt pct Ni}] \quad [16e]$$

$$\log^{\alpha} K_{\mathrm{VN}} - \log^{\alpha}K^{0}_{\mathrm{VN}} \cong \left(-0.05 + \frac{85}{T}\right)[\text{wt pct Mn}] + \left(-0.03 + \frac{49}{T}\right)[\text{wt pct Ni}] \quad [16f]$$

IV. DISCUSSION

Thermodynamic calculations to evaluate solubility products of titanium, niobium, vanadium carbide, and nitride in ferrite under the effect of solid solution alloy elements Mn and Ni are based on four assumptions in the present work. The four assumptions actually are reasonable in applications: (a) the two sublattice model is a general model adopted by previous studies for thermodynamic calculation;[7,11,12] (b) solubilities of C and N in pure iron are tiny[13,14] and Ti, Nb, and V are usually added to steels as microalloy elements; (c) the thermodynamic parameters used in the present calculations in Tables AI through AII actually match assumption [3]; and (d) assumption [4] is a common principle used in thermodynamics.[15] Therefore, on the condition that the total content of solid solution elements in ferrite is relatively small (probably less than about 10 wt pct), thermodynamic calculations in the present work are available to deduce the solubility products of titanium, niobium, vanadium carbide, and nitride in ferrite. In particular, assumptions [1] and [4] are more like a universal principle in thermodynamic calculations and assumption [3] is a widespread phenomenon. Therefore, if assumption [2] is satisfied, the solubility products of other fcc binary compounds in ferrite also can be evaluated with the thermodynamic models in the present work.

All the thermodynamic parameters used for solubility product calculations in Tables AI through AIII are quoted from published documents. The data source of Gibbs energies in the documents originates from the thermodynamic data manual.[16–18] Thermodynamic interaction parameters of $L^{\mathrm{bcc}}_{\mathrm{Fe},M:\mathrm{Va}}$, $L^{\mathrm{bcc}}_{\mathrm{Fe}:N,\mathrm{Va}}$, ${}^{0}T^{\mathrm{bcc}}_{c\mathrm{Fe}}$, ${}^{0}T^{\mathrm{bcc}}_{c\mathrm{Fe},M}$, ${}^{0}\beta^{\mathrm{bcc}}_{\mathrm{Fe}}$, and ${}^{0}\beta^{\mathrm{bcc}}_{\mathrm{Fe},M}$ are preferentially referenced from investigations on the solubility of carbonitrides in the Fe-V-C-N,[8] Fe-Nb-C-N,[19] and Fe-Ti-C-N[20] systems and supplemented from investigations on the thermodynamic analysis of the Fe-N phase diagram[21] and Fe-Ti-V system.[10] Parameters of $L^{\mathrm{bcc}}_{\mathrm{Fe},X_i:\mathrm{Va}}$, $L^{\mathrm{bcc}}_{\mathrm{Fe},X_i:N}$, ${}^{0}T^{\mathrm{bcc}}_{cX_i}$, ${}^{0}T^{\mathrm{bcc}}_{c\mathrm{Fe},X_i}$, and ${}^{0}\beta^{\mathrm{bcc}}_{X_i}$ are preferentially referenced from investigations on thermodynamic assessment of the Fe-Mn-N,[22] Fe-Cr-Ni-C,[23] and Fe-Mn-C[24] systems and supplemented from the investigation on

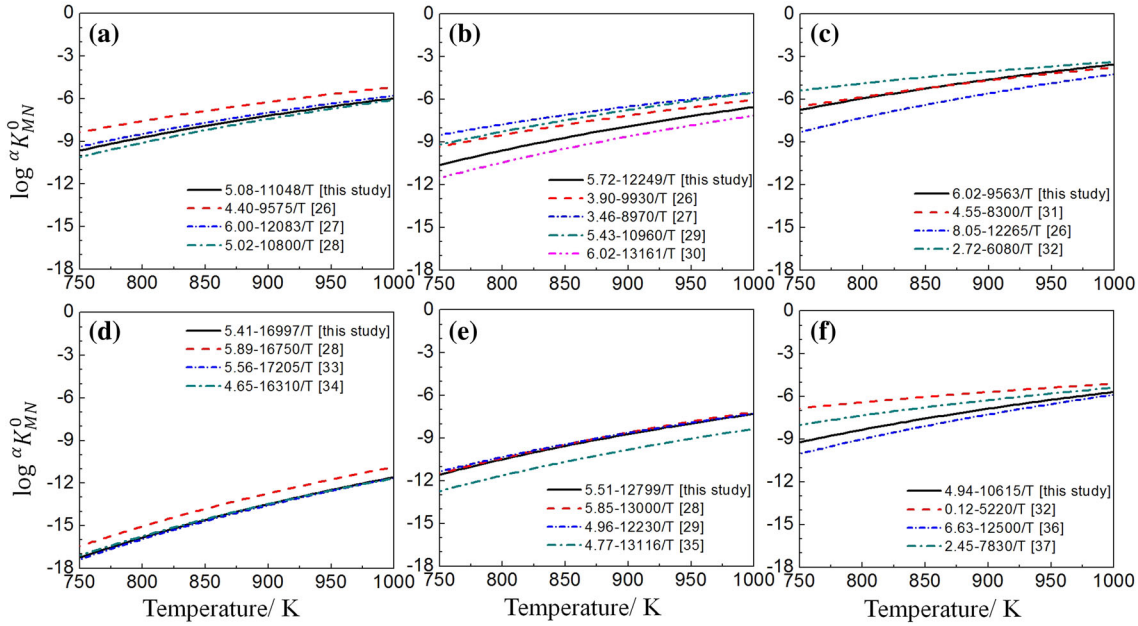

Fig. 4—Comparisons of solubility products of carbides and nitrides in pure ferrite in this study with those in previous studies: (*a*) TiC, (*b*) NbC, (*c*) VC, (*d*) TiN, (*e*) NbN, and (*f*) VN.

thermodynamic analysis of the Fe-Ni-Cr-Mo-C-N system.[25] Therefore, it is considered that the thermodynamic interaction parameters in the Appendix are valid for the composition region in the current calculation.

Many previous researchers have studied the solubility products of these carbides and nitrides in ferrite using thermodynamic calculations or experiment measurements, of which results are summarized in Table I. Comparisons of solubility products in pure ferrite in this study with those in previous studies are seen in Figure 4, showing that the utmost difference of solubility products of each binary compound is at low temperatures, which is within about three orders of magnitude. The solubility products in Table I, developed from thermodynamic calculations, are mainly based on two models: the solution model[26,33,35] and the two sublattice model.[27,28,34,36] Obvious characteristics in previous studies are (a) some terms in describing Gibbs energy of ferrite were ignored in their models[26,33,35,36] and (b) some thermodynamic parameters were missed in their calculations[26–28,34–36] for lack of thermodynamic data at that time. However, the developed solubility products in previous studies are also reliable and keep good agreement with the experimental data for large terms in the models and calculations. With the developments in computer coupling of phase diagrams and thermochemistry (CALPHAD) in the recent decade, most of the missed thermodynamic parameters in previous thermodynamic calculations under the two sublattice model have been determined. Taking in consideration of all the referenced thermodynamic parameters in our thermodynamic calculations, it is believed our calculations can give a much more accuracy in comparative of previous calculations. What a clear demarcation can be seen in Figure 4(c), (d), and (f) that the calculated solubility products of VC, TiN, and VN in this study are closer to the solubility products by experimental measurements (especially in the experiment measurement temperature ranges[31,32]) than the solubility products by thermodynamic calculations in previous studies, which states that the calculated results in this study can be considered reliably as can the studies on the effect of solid solution elements on the solubility products of these carbides and nitrides in ferrite.

V. CONCLUSIONS

Thermodynamic calculations are used to evaluate solubility products of fcc binary compound in ferrite in the present work. With submitting the thermodynamic parameters from the references herein, the solubility products of titanium, niobium, vanadium carbide, and nitride in ferrite under the effect of solid solution alloy elements Mn and Ni are studied. The results show that the calculated solubility products of these binary compounds in pure ferrite are closer to the solubility products by experimental measurements than the solubility products by thermodynamic calculations in previous studies. The solid solution element of Mn or Ni can result in an increase in these solubility products, but the increments would limit in 0.8 orders of magnitude even when the content of Mn or Ni is 10 wt pct.

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APPENDIX

$$\begin{aligned}\frac{\partial G^{\alpha}}{\partial y^{\alpha}_{\mathrm{Fe}}} &= y^{\alpha}_{N}{}^{\circ}G^{\mathrm{bcc}}_{\mathrm{Fe:N}} + y^{\alpha}_{\mathrm{Va}}{}^{\circ}G^{\mathrm{bcc}}_{\mathrm{Fe:Va}} + RT(\ln y^{\alpha}_{\mathrm{Fe}} + 1)\\ &+ y^{\alpha}_{N}y^{\alpha}_{\mathrm{Va}}L^{\mathrm{bcc}}_{\mathrm{Fe}:N,\mathrm{Va}} + y^{\alpha}_{M}y^{\alpha}_{N}L^{\mathrm{bcc}}_{\mathrm{Fe},M:N} + y^{\alpha}_{M}y^{\alpha}_{\mathrm{Va}}L^{\mathrm{bcc}}_{\mathrm{Fe,M:Va}}\\ &+ \sum_{i} y^{\alpha}_{X_i}y^{\alpha}_{N}L^{\mathrm{bcc}}_{\mathrm{Fe},X_i:N} + \sum_{i} y^{\alpha}_{X_i}y^{\alpha}_{\mathrm{Va}}L^{\mathrm{bcc}}_{\mathrm{Fe},X_i:\mathrm{Va}}\\ &- RT\ln\left(\beta^{\mathrm{bcc}}+1\right)\frac{\mathrm{d}f(\tau)}{\mathrm{d}\tau}\frac{\tau}{T^{\mathrm{bcc}}_{c}}\\ &\times\left[{}^{0}T^{\mathrm{bcc}}_{c\mathrm{Fe}} + \sum_{i} y^{\alpha}_{X_i}\sum_{n} nT^{\mathrm{bcc}}_{c\mathrm{Fe},X_i}\left(y^{\alpha}_{\mathrm{Fe}} - y^{\alpha}_{X_i}\right)^{n}\right.\\ &+ \sum_{i} y^{\alpha}_{\mathrm{Fe}}y^{\alpha}_{X_i}\sum_{n} nnT^{\mathrm{bcc}}_{c\mathrm{Fe},X_i}\left(y^{\alpha}_{\mathrm{Fe}} - y^{\alpha}_{X_i}\right)^{n-1}\\ &+ y^{\alpha}_{M}\sum_{n} nT^{\mathrm{bcc}}_{c\mathrm{Fe,M}}\left(y^{\alpha}_{\mathrm{Fe}} - y^{\alpha}_{M}\right)^{n}\\ &\left.+ y^{\alpha}_{\mathrm{Fe}}y^{\alpha}_{M}\sum_{n} nnT^{\mathrm{bcc}}_{\mathrm{cFe,M}}\left(y^{\alpha}_{\mathrm{Fe}} - y^{\alpha}_{M}\right)^{n-1}\right]\\ &+ RTf(\tau)\frac{1}{\beta^{\mathrm{bcc}}+1}\\ &\times\left[{}^{0}\beta^{\mathrm{bcc}}_{Fe} + \sum_{i} y^{\alpha}_{X_i}\sum_{n} n\beta^{\mathrm{bcc}}_{\mathrm{Fe},X_i}\left(y^{\alpha}_{\mathrm{Fe}} - y^{\alpha}_{X_i}\right)^{n}\right.\\ &+ \sum_{i} y^{\alpha}_{\mathrm{Fe}}y^{\alpha}_{X_i}\sum_{n} nn\beta^{\mathrm{bcc}}_{\mathrm{Fe},X_i}\left(y^{\alpha}_{\mathrm{Fe}} - y^{\alpha}_{X_i}\right)^{n-1}\\ &+ y^{\alpha}_{M}\sum_{n} n\beta^{\mathrm{bcc}}_{\mathrm{Fe},M}\left(y^{\alpha}_{\mathrm{Fe}} - y^{\alpha}_{M}\right)^{n}\\ &\left.+ y^{\alpha}_{\mathrm{Fe}}y^{\alpha}_{M}\sum_{n} nn\beta^{\mathrm{bcc}}_{\mathrm{Fe},M}\left(y^{\alpha}_{\mathrm{Fe}} - y^{\alpha}_{M}\right)^{n-1}\right]\end{aligned} \tag{A1a}$$

$$\begin{aligned}\frac{\partial G^{\alpha}}{\partial y^{\alpha}_{X_i}} &= y^{\alpha}_{N}{}^{\circ}G^{\mathrm{bcc}}_{X_i:N} + y^{\alpha}_{\mathrm{Va}}{}^{\circ}G^{\mathrm{bcc}}_{X_i:\mathrm{Va}} + RT\left(\ln y^{\alpha}_{X_i} + 1\right)\\ &+ y^{\alpha}_{N}y^{\alpha}_{\mathrm{Va}}L^{\mathrm{bcc}}_{X_i:N,\mathrm{Va}} + y^{\alpha}_{\mathrm{Fe}}y^{\alpha}_{N}L^{\mathrm{bcc}}_{\mathrm{Fe,X_i:N}}\\ &+ \sum_{i'} y^{\alpha}_{X_{i'}}y^{\alpha}_{N}L^{\mathrm{bcc}}_{X_{i'},X_i:N} + y^{\alpha}_{M}y^{\alpha}_{N}L^{\mathrm{bcc}}_{X_i,M:N}\\ &+ y^{\alpha}_{\mathrm{Fe}}y^{\alpha}_{\mathrm{Va}}L^{\mathrm{bcc}}_{\mathrm{Fe,X_i:Va}} + \sum_{i'} y^{\alpha}_{X_{i'}}y^{\alpha}_{\mathrm{Va}}L^{\mathrm{bcc}}_{X_{i'},X_i:\mathrm{Va}}\\ &+ y^{\alpha}_{M}y^{\alpha}_{N}L^{\mathrm{bcc}}_{X_i,M:\mathrm{Va}} - RT\ln\left(\beta^{\mathrm{bcc}}+1\right)\frac{\mathrm{d}f(\tau)}{\mathrm{d}\tau}\frac{\tau}{T^{\mathrm{bcc}}_{c}}\\ &\times\left[{}^{0}T^{\mathrm{bcc}}_{cX_i} + y^{\alpha}_{\mathrm{Fe}}\sum_{n} nT^{\mathrm{bcc}}_{c\mathrm{Fe},X_i}\left(y^{\alpha}_{Fe} - y^{\alpha}_{X_i}\right)^{n}\right.\\ &- y^{\alpha}_{\mathrm{Fe}}y^{\alpha}_{X_i}\sum_{n} nnT^{\mathrm{bcc}}_{c\mathrm{Fe},X_i}\left(y^{\alpha}_{\mathrm{Fe}} - y^{\alpha}_{X_i}\right)^{n-1}\\ &+ \sum_{i'} y^{\alpha}_{X_{i'}}\sum_{n} nT^{\mathrm{bcc}}_{cX_i,X_i}\left(y^{\alpha}_{X_i} - y^{\alpha}_{X_{i'}}\right)^{n}\\ &+ \sum_{i'} y^{\alpha}_{X_i}y^{\alpha}_{X_{i'}}\sum_{n} nnT^{\mathrm{bcc}}_{cX_i,X_i}\left(y^{\alpha}_{X_i} - y^{\alpha}_{X_{i'}}\right)^{n-1}\\ &+ y^{\alpha}_{M}\sum_{n} nT^{\mathrm{bcc}}_{cX_i,M}\left(y^{\alpha}_{X_i} - y^{\alpha}_{M}\right)^{n}\\ &\left.+ y^{\alpha}_{X_i}y^{\alpha}_{M}\sum_{n} nnT^{\mathrm{bcc}}_{cX_i,M}\left(y^{\alpha}_{X_i} - y^{\alpha}_{M}\right)^{n-1}\right]\\ &+ RTf(\tau)\frac{1}{\beta^{bcc}+1}\left[{}^{0}\beta^{\mathrm{bcc}}_{X_i} + y^{\alpha}_{Fe}\sum_{n} n\beta^{\mathrm{bcc}}_{\mathrm{Fe},X_i}\left(y^{\alpha}_{\mathrm{Fe}} - y^{\alpha}_{X_i}\right)^{n}\right.\\ &- y^{\alpha}_{Fe}y^{\alpha}_{X_i}\sum_{n} nn\beta^{\mathrm{bcc}}_{\mathrm{Fe},X_i}\left(y^{\alpha}_{Fe} - y^{\alpha}_{X_i}\right)^{n-1}\\ &+ \sum_{i'} y^{\alpha}_{X_{i'}}\sum_{n}{}^{n}\beta^{\mathrm{bcc}}_{X_i,X_i}\left(y^{\alpha}_{X_i} - y^{\alpha}_{X_{i'}}\right)^{n}\\ &+ \sum_{i'} y^{\alpha}_{X_i}y^{\alpha}_{X_{i'}}\sum_{n} nn\beta^{\mathrm{bcc}}_{X_i,X_i}\left(y^{\alpha}_{X_i} - y^{\alpha}_{X_{i'}}\right)^{n-1}\\ &+ y^{\alpha}_{M}\sum_{n} n\beta^{\mathrm{bcc}}_{X_i,M}\left(y^{\alpha}_{X_i} - y^{\alpha}_{M}\right)^{n}\\ &\left.+ y^{\alpha}_{X_i}y^{\alpha}_{M}\sum_{n} nn\beta^{\mathrm{bcc}}_{X_i,M}\left(y^{\alpha}_{X_i} - y^{\alpha}_{M}\right)^{n-1}\right]\end{aligned} \tag{A1b}$$

Table AI. Thermodynamic Parameters of Gibbs Energies

Gibbs Energy (J/mol)	Ref.
${}^{\circ}G^{\mathrm{bcc}}_{\mathrm{Fe:C}} - {}^{\circ}G^{\mathrm{bcc}}_{\mathrm{Fe:Va}} - 3{}^{\circ}G^{\mathrm{gra}}_{\mathrm{C}} = 322,050 + 75.667\,T$	8
${}^{\circ}G^{\mathrm{bcc}}_{\mathrm{Fe:N}} - {}^{\circ}G^{\mathrm{bcc}}_{\mathrm{Fe:Va}} - 3{}^{\circ}G^{\mathrm{gas}}_{\mathrm{N}} = 93,562 + 165.07T$	8
${}^{\circ}G^{\mathrm{bcc}}_{\mathrm{Mn:C}} - {}^{\circ}G^{\mathrm{bcc}}_{\mathrm{Mn:Va}} - 3{}^{\circ}G^{\mathrm{gra}}_{\mathrm{C}} = -4879.98 + 32.209T + 0.2418T\ln\,T + 9.502 \times 10^{-5}T^2 + 9827/T$	23, 38
${}^{\circ}G^{\mathrm{bcc}}_{\mathrm{Mn:N}} - {}^{\circ}G^{\mathrm{bcc}}_{\mathrm{Mn:Va}} - 3{}^{\circ}G^{\mathrm{gas}}_{\mathrm{N}} = -41,112.675 + 507.16075T - 38.3643T\ln T - 7.972758 \times 10^{-3}T^2 - 8.043 \times 10^{-9}T^3$	22
$+ 882,019/T, 298 \le T \le 950; = -30,288.15 + 427.1971T - 27.6003T\ln\,T + 9.3978 \times 10^{-3}T^2$	
$- 9.0291 \times 10^{-8}T^3 - 904,313/T, 950 < T < 1519$	
${}^{\circ}G^{\mathrm{bcc}}_{\mathrm{Ni:C}} - {}^{\circ}G^{\mathrm{bcc}}_{\mathrm{Ni:Va}} - 3{}^{\circ}G^{\mathrm{gra}}_{\mathrm{C}} = 400,000 - 100T$	23
${}^{\circ}G^{\mathrm{bcc}}_{\mathrm{Ni:N}} - {}^{\circ}G^{\mathrm{bcc}}_{\mathrm{Ni:Va}} - 3{}^{\circ}G^{\mathrm{gas}}_{\mathrm{N}} = 202,569 + 420.62T - 32.7231T\ln T$	25
${}^{\circ}G^{\mathrm{fcc}}_{\mathrm{Ti:C}} - {}^{\circ}G^{\mathrm{bcc}}_{\mathrm{Ti:Va}} - {}^{\circ}G^{\mathrm{gra}}_{\mathrm{C}} = -149,837.079 - 6.753408T + 0.2738T\ln\,T + 2.530275 \times 10^{-3}T^2 - 1.08746 \times 10^{-7}T^3$	20, 39
$- 1,816,236/T + 2.643 \times 10^{8}T^{-2} - 1.2 \times 10^{10}T^{-3}, 298 \le T \le 900; = -150,085.185 - 6.126268T + 0.2692T\ln\,T$	
$+ 1.9556 \times 10^{-3}T^2 - 9.2906 \times 10^{-8}T^3 - 1,786,280/T + 2.643 \times 10^{8}T^{-2} - 1.2 \times 10^{10}T^{-3}, 900 \le T \le 1155$	
${}^{\circ}G^{\mathrm{fcc}}_{\mathrm{Ti:N}} - {}^{\circ}G^{\mathrm{bcc}}_{\mathrm{Ti:Va}} - {}^{\circ}G^{\mathrm{gas}}_{\mathrm{N}} = -163,445.404 + 173.430842T - 11.2443T\ln\,T + 2.234661 \times 10^{-3}T^2 - 1.11427 \times 10^{-7}T^3 + 778,738/T, 298 \le T < 900$	
$= -163,703.51 + 174.057982T - 11.2489T\ln\,T + 1.659986 \times 10^{-3}T^2 - 9.5587 \times 10^{-8}T^3 + 808,694/T, 900 \le T < 950$	20, 22, 39, 40
$= -160,095.335 + 147.403432T - 7.6609T\ln\,T + 2.135 \times 10^{-3}T^2 - 1.23003 \times 10^{-7}T^3 + 213,250/T, 950 \le T < 1155$	
${}^{\circ}G^{\mathrm{fcc}}_{\mathrm{Nb:C}} - {}^{\circ}G^{\mathrm{bcc}}_{\mathrm{Nb:Va}} - {}^{\circ}G^{\mathrm{gra}}_{\mathrm{C}} = -155,650 - 5.31T$	41, 42
${}^{\circ}G^{\mathrm{fcc}}_{\mathrm{Nb:N}} - {}^{\circ}G^{\mathrm{bcc}}_{\mathrm{Nb:Va}} - {}^{\circ}G^{\mathrm{gas}}_{\mathrm{N}} = -245,775 + 113.411T - 4T\ln\,T$	19, 41, 42
${}^{\circ}G^{\mathrm{fcc}}_{\mathrm{V:C}} - {}^{\circ}G^{\mathrm{bcc}}_{\mathrm{V:Va}} - {}^{\circ}G^{\mathrm{gra}}_{\mathrm{C}} = -108,465.158 - 56.707093T + 8.444T\ln T + 5.98081 \times 10^{-3}T^2 + 6.8 \times 10^{-7}T^3 - 1,972,054/T$	8, 38, 39
$+ 2.643 \times 10^{8}T^{-2} - 1.2 \times 10^{10}T^{-3}$	
${}^{\circ}G^{\mathrm{fcc}}_{\mathrm{V:N}} - {}^{\circ}G^{\mathrm{bcc}}_{\mathrm{V:Va}} - {}^{\circ}G^{\mathrm{gas}}_{\mathrm{N}} = -122,083.483 + 123.477157T - 3.0741T\ln T + 5.685196 \times 10^{-3}T^2 + 6.77319 \times 10^{-7}T^3$	8, 22
$+ 622,920/T, 298 \le T < 950 = -118,475 + 96.822607T + 0.5139T\ln T - 6.16021$	
$\times 10^{-3}T^2 + 6.49903 \times 10^{-7}T^3 + 27,476/T, 950 \le T < 3300$	

Table AII. Thermodynamic Interaction Parameters

Interaction Parameter (J/mol)	Ref.
$L^{\mathrm{bcc}}_{\mathrm{Fe:C,Va}} = -190T$	20
$L^{\mathrm{bcc}}_{\mathrm{Fe:N,Va}} = 0$	21
$L^{\mathrm{bcc}}_{\mathrm{Fe,Mn:Va}} = -2759 + 1.237T$	22
$L^{\mathrm{bcc}}_{\mathrm{Fe,Ni:Va}} = -956.63 - 1.28726T + (1789.03 - 1.92912T)(y^{\alpha}_{\mathrm{Fe}} - y^{\alpha}_{\mathrm{Ni}})$	23
$L^{\mathrm{bcc}}_{\mathrm{Fe,Ti:Va}} = -59,098 + 11.5T - (3906 + 4.5T)(y^{\alpha}_{\mathrm{Ti}} - y^{\alpha}_{\mathrm{Fe}})$	19
$L^{\mathrm{bcc}}_{\mathrm{Fe,Nb:Va}} = -25,373 + 17.1886T$	20
$L^{\mathrm{bcc}}_{\mathrm{Fe,V:Va}} = -23,674 + 0.465T + 8283(y^{\alpha}_{\mathrm{Fe}} - y^{\alpha}_{\mathrm{V}})$	8
$L^{\mathrm{bcc}}_{\mathrm{Mn:C,Va}} = -62.9012T$	24
$L^{\mathrm{bcc}}_{\mathrm{Ni:C,Va}} = 0$	25
$L^{\mathrm{bcc}}_{\mathrm{Mn:N,Va}} = -185,000$	22
$L^{\mathrm{bcc}}_{\mathrm{Ni:N,Va}}$	missed
$L^{\mathrm{bcc}}_{\mathrm{Fe,Mn:C}} = 34,052 - 23.467T$	24
$L^{\mathrm{bcc}}_{\mathrm{Fe,Ni:C}} = -956.63 - 1.28726T + (1789.03 - 1.92912T)(y^{\alpha}_{\mathrm{Fe}} - y^{\alpha}_{\mathrm{Ni}})$	23
$L^{\mathrm{bcc}}_{\mathrm{Fe,Mn:N}}$	missed
$L^{\mathrm{bcc}}_{\mathrm{Fe,Ni:N}} = 580 - 5.327T$	25

Table AIII. Thermodynamic Interaction Parameters for Magnetic Contribution

Parameter	Ref.
${}^{0}T^{\mathrm{bcc}}_{c\mathrm{Fe}} = 1043K$	8, 22
${}^{0}T^{\mathrm{bcc}}_{c\mathrm{Ni}} = 575K$	23
${}^{0}T^{\mathrm{bcc}}_{c\mathrm{Fe,Mn}} = 123K$	22
${}^{0}T^{\mathrm{bcc}}_{c\mathrm{Fe,Ti}} = 637.79K$	10
${}^{0}T^{\mathrm{bcc}}_{c\mathrm{Fe,V}} = -110K$	8, 10
${}^{1}T^{\mathrm{bcc}}_{c\mathrm{Fe,V}} = 3075K$	8, 10
${}^{2}T^{\mathrm{bcc}}_{c\mathrm{Fe,V}} = 808K$	8, 10
${}^{3}T^{\mathrm{bcc}}_{c\mathrm{Fe,V}} = -2169K$	8, 10
${}^{0}\beta^{\mathrm{bcc}}_{\mathrm{Fe}} = 2.22$	8
${}^{0}\beta^{\mathrm{bcc}}_{\mathrm{Mn}} = -0.27$	22
${}^{0}\beta^{\mathrm{bcc}}_{\mathrm{Ni}} = 0.85$	25
${}^{0}\beta^{\mathrm{bcc}}_{\mathrm{Fe,V}} = -2.26$	8, 38

$$\begin{aligned}\frac{\partial G^{\alpha}}{\partial y^{\alpha}_{M}} &= y^{\alpha}_{N}\,{}^{\circ}G^{\mathrm{bcc}}_{M:N} + y^{\alpha}_{\mathrm{Va}}\,{}^{\circ}G^{\mathrm{bcc}}_{M:\mathrm{Va}} + RT(\ln y^{\alpha}_{M} + 1) \\ &+ y^{\alpha}_{N}y^{\alpha}_{\mathrm{Va}}L^{\mathrm{bcc}}_{M:N,\mathrm{Va}} + y^{\alpha}_{\mathrm{Fe}}y^{\alpha}_{N}L^{\mathrm{bcc}}_{\mathrm{Fe,M:N}} + y^{\alpha}_{\mathrm{Fe}}y^{\alpha}_{\mathrm{Va}}L^{\mathrm{bcc}}_{\mathrm{Fe,M:Va}} \\ &+ \sum_{i} y^{\alpha}_{X_i}y^{\alpha}_{N}L^{\mathrm{bcc}}_{X_i,M:N} + \sum_{i} y^{\alpha}_{X_i}y^{\alpha}_{\mathrm{Va}}L^{\mathrm{bcc}}_{X_i,M:\mathrm{Va}} \\ &- RT\ln(\beta^{\mathrm{bcc}} + 1)\frac{\mathrm{d}f(\tau)}{\mathrm{d}\tau}\frac{\tau}{T^{\mathrm{bcc}}_{c}} \\ &\times \left[{}^{0}T^{\mathrm{bcc}}_{cM} + y^{\alpha}_{\mathrm{Fe}}\sum_{n}{}^{n}T^{\mathrm{bcc}}_{c\mathrm{Fe},M}(y^{\alpha}_{\mathrm{Fe}} - y^{\alpha}_{M})^{n}\right. \\ &- y^{\alpha}_{\mathrm{Fe}}y^{\alpha}_{M}\sum_{n} n\,{}^{n}T^{\mathrm{bcc}}_{c\mathrm{Fe},M}(y^{\alpha}_{\mathrm{Fe}} - y^{\alpha}_{M})^{n-1} \\ &+ \sum_{i} y^{\alpha}_{X_i}\sum_{n}{}^{n}T^{\mathrm{bcc}}_{cX_i,M}\left(y^{\alpha}_{X_i} - y^{\alpha}_{M}\right)^{n} \\ &\left.- \sum_{i} y^{\alpha}_{X_i}y^{\alpha}_{M}\sum_{n} n\,{}^{n}T^{\mathrm{bcc}}_{cX_i,M}\left(y^{\alpha}_{X_i} - y^{\alpha}_{M}\right)^{n-1}\right] \\ &+ RTf(\tau)\frac{1}{\beta^{\mathrm{bcc}} + 1}\left[{}^{0}\beta^{\mathrm{bcc}}_{M} + y^{\alpha}_{\mathrm{Fe}}\sum_{n}{}^{n}\beta^{\mathrm{bcc}}_{\mathrm{Fe},M}(y^{\alpha}_{\mathrm{Fe}} - y^{\alpha}_{M})^{n}\right. \\ &- y^{\alpha}_{\mathrm{Fe}}y^{\alpha}_{M}\sum_{n} n^{n}\beta^{\mathrm{bcc}}_{\mathrm{Fe},M}(y^{\alpha}_{Fe} - y^{\alpha}_{M})^{n-1} \\ &+ \sum_{i} y^{\alpha}_{X_i}\sum_{n}{}^{n}\beta^{\mathrm{bcc}}_{X_i,M}\left(y^{\alpha}_{X_i} - y^{\alpha}_{M}\right)^{n} \\ &\left.- \sum_{i} y^{\alpha}_{X_i}y^{\alpha}_{M}\sum_{n} n^{n}\beta^{\mathrm{bcc}}_{X_i,M}\left(y^{\alpha}_{X_i} - y^{\alpha}_{M}\right)^{n-1}\right] \end{aligned} \quad [A1c]$$

$$\begin{aligned}\frac{\partial G^{\alpha}}{\partial y^{\alpha}_{N}} &= y^{\alpha}_{\mathrm{Fe}}\,{}^{\circ}G^{\mathrm{bcc}}_{Fe:N} + \sum_{i} y^{\alpha}_{X_i}\,{}^{\circ}G^{\mathrm{bcc}}_{X_i:N} + y^{\alpha}_{M}\,{}^{\circ}G^{\mathrm{bcc}}_{M:N} \\ &+ 3RT(\ln y^{\alpha}_{N} + 1) + y^{\alpha}_{\mathrm{Fe}}y^{\alpha}_{Va}L^{\mathrm{bcc}}_{Fe:N,Va} \\ &+ \sum_{i} y^{\alpha}_{X_i}y^{\alpha}_{Va}L^{\mathrm{bcc}}_{X_i:N,Va} + y^{\alpha}_{M}y^{\alpha}_{Va}L^{\mathrm{bcc}}_{M:N,Va} \\ &+ \sum_{i} y^{\alpha}_{\mathrm{Fe}}y^{\alpha}_{X_i}L^{\mathrm{bcc}}_{Fe,X_i:N} + \sum_{i} y^{\alpha}_{X_i}\sum_{i'} y^{\alpha}_{X_{i'}}L^{\mathrm{bcc}}_{X_i,X_{i'}:N} \\ &+ \sum_{i} y^{\alpha}_{X_i}y^{\alpha}_{M}L^{\mathrm{bcc}}_{X_i,M:N} + y^{\alpha}_{\mathrm{Fe}}y^{\alpha}_{M}L^{\mathrm{bcc}}_{Fe,M:N} \end{aligned} \quad [A1d]$$

$$\frac{\partial G^{\alpha}}{\partial y^{\alpha}_{\mathrm{Va}}} = y^{\alpha}_{\mathrm{Fe}}\,{}^{\circ}G^{\mathrm{bcc}}_{\mathrm{Fe:Va}} + \sum_i y^{\alpha}_{X_i}\,{}^{\circ}G^{\mathrm{bcc}}_{\mathrm{X_i:Va}} + y^{\alpha}_{M}\,{}^{\circ}G^{\mathrm{bcc}}_{M:Va} + 3RT\left(\ln y^{\alpha}_{\mathrm{Va}} + 1\right) + y^{\alpha}_{\mathrm{Fe}} y^{\alpha}_{N} L^{\mathrm{bcc}}_{\mathrm{Fe:N,Va}} + \sum_i y^{\alpha}_{X_i} y^{\alpha}_{N} L^{\mathrm{bcc}}_{X_i:N,\mathrm{Va}} + y^{\alpha}_{M} y^{\alpha}_{N} L^{\mathrm{bcc}}_{M:N,\mathrm{Va}} + \sum_i y^{\alpha}_{\mathrm{Fe}} y^{\alpha}_{X_i} L^{bcc}_{\mathrm{Fe},X_i:\mathrm{Va}} + \sum_i y^{\alpha}_{X_i} \sum_{i'} y^{\alpha}_{X_{i'}} L^{bcc}_{X_i,X_{i'}:\mathrm{Va}} + \sum_i y^{\alpha}_{X_i} y^{\alpha}_{M} L^{\mathrm{bcc}}_{X_i,M:\mathrm{Va}} + y^{\alpha}_{\mathrm{Fe}} y^{\alpha}_{M} L^{\mathrm{bcc}}_{\mathrm{Fe,M:Va}} \quad [A1e]$$

The term ${}^{mg}\mu^{\mathrm{bcc}}_{M}$ is usually very small compared with the term ΔG_{MN} in Eq. [9]; it is not considered in the approximation of Eq. [13]. Thus, $\Delta\log {}^{\alpha}K^{X_1}_{MN}$ can be approximated as

$$\Delta\log^{\alpha}K^{X_1}_{MN} = \log {}^{\alpha}K^{X_1}_{MN} - \log^{\alpha}K^{0}_{MN} \cong \left[\Delta G^{\alpha}_{MN}(x_{\mathrm{Fe}}, x_{X_1}, 0, \cdots) - \Delta G_{MN}(1,0,0,\cdots)\right] \Big/ RT\ln 10 + \log\frac{A^2_{\mathrm{Fe}}}{\left[A_{\mathrm{Fe}}(1-x_{X_i}) + x_{X_i}A_{X_i}\right]^2} \quad [A2a]$$

$$\begin{aligned}
&\Delta G^{\alpha}_{MN}(x_{\mathrm{Fe}}, x_{X_1}, 0, \cdots) - \Delta G^{\alpha}_{MN}(1,0,0,\cdots)\\
&\cong \Delta G^{\alpha}_{MN}(1-x_{X_1}, x_{X_1}, 0, \cdots) - \Delta G^{\alpha}_{MN}(1,0,0,\cdots)\\
&= x_{X_1}\left({}^{\circ}G^{\mathrm{bcc}}_{\mathrm{Fe:N}} - {}^{\circ}G^{\mathrm{bcc}}_{\mathrm{Fe:Va}}\right)\Big/3 - x_{X_1}\left({}^{\circ}G^{\mathrm{bcc}}_{X_1:N} - {}^{\circ}G^{\mathrm{bcc}}_{X_1:Va}\right)\Big/3\\
&\quad + x_{X_1}L^{\mathrm{bcc}}_{Fe,M:Va} + x_{X_1}L^{\mathrm{bcc}}_{X_1,M:\mathrm{Va}} + x_{X_1}L^{\mathrm{bcc}}_{\mathrm{Fe},X_1:\mathrm{Va}}\\
&\quad - \left(x_{X_1}L^{\mathrm{bcc}}_{X_1:\mathrm{N,Va}} - x_{X_1}L^{\mathrm{bcc}}_{\mathrm{Fe:N,Va}}\right)\Big/3\\
&\quad - x_{X_1}\left(L^{\mathrm{bcc}}_{\mathrm{Fe},X_1:N} - L^{\mathrm{bcc}}_{\mathrm{Fe},X_1:\mathrm{Va}}\right)\Big/3 - x_{X_1}x_{X_1}L^{\mathrm{bcc}}_{\mathrm{Fe},X_1:\mathrm{Va}}\\
&\quad + x_{X_1}x_{X_1}\left(L^{\mathrm{bcc}}_{\mathrm{Fe},X_1:N} - L^{\mathrm{bcc}}_{\mathrm{Fe},X_1:\mathrm{Va}}\right)\Big/3
\end{aligned} \quad [A2b]$$

The following relationship is given as

$$\log^{\alpha}K_{MN} - \log^{\alpha}K^{0}_{MN} \cong \left[\Delta G^{\alpha}_{MN}(x_{\mathrm{Fe}}, x_{X_1}, x_{X_2}, \cdots) - \Delta G^{\alpha}_{MN}(1,0,0,\cdots)\right] \Big/ \mathrm{R}T\ln 10 + \log\frac{A^2_{\mathrm{Fe}}}{\left[A_{\mathrm{Fe}}\left(1-\sum_i x_{X_i}\right) + \sum_i x_{X_i}A_{X_i}\right]^2} \quad [A3a]$$

With considering the total content of solid solution elements in ferrite is relatively small, the following approximations are established.

$$\begin{aligned}
&\Delta G^{\alpha}_{MN}(x_{\mathrm{Fe}}, x_{X_1}, x_{X_2}, \cdots) - \Delta G^{\alpha}_{MN}(1,0,0,\cdots)\\
&\cong \Delta G^{\alpha}_{MN}(1-\sum_i x_{X_i}, x_{X_1}, x_{X_2}, \cdots) - \Delta G^{\alpha}_{MN}(1,0,0,\cdots)\\
&= \sum_i x_{X_1}\left({}^{\circ}G^{\mathrm{bcc}}_{\mathrm{Fe:N}} - {}^{\circ}G^{\mathrm{bcc}}_{\mathrm{Fe:Va}}\right)\Big/3\\
&\quad - \sum_i x_{X_i}\left({}^{\circ}G^{\mathrm{bcc}}_{X_i:N} - {}^{\circ}G^{\mathrm{bcc}}_{X_i:\mathrm{Va}}\right)\Big/3 + \sum_i x_{X_i}L^{\mathrm{bcc}}_{\mathrm{Fe},M:\mathrm{Va}}\\
&\quad - \sum_i x_{X_i}L^{\mathrm{bcc}}_{X_i,M:\mathrm{Va}} + \sum_i x_{X_1}L^{\mathrm{bcc}}_{\mathrm{Fe,X_i:Va}}\\
&\quad - \left(\sum_i x_{X_1}L^{\mathrm{bcc}}_{X_i:N,Va} - \sum_i x_{X_1}L^{\mathrm{bcc}}_{\mathrm{Fe:N,Va}}\right)\Big/3\\
&\quad - \sum_i x_{X_1}\left(L^{\mathrm{bcc}}_{\mathrm{Fe},X_i:N} - L^{\mathrm{bcc}}_{\mathrm{Fe},X_i:\mathrm{Va}}\right)\Big/3\\
&\quad - \sum_i x_{X_i}\sum_i x_{X_i}L^{\mathrm{bcc}}_{\mathrm{Fe},X_1:\mathrm{Va}}\\
&\quad + \sum_i x_{X_i}\sum_i x_{X_i}\left(L^{\mathrm{bcc}}_{\mathrm{Fe},X_1:N} - L^{\mathrm{bcc}}_{\mathrm{Fe},X_1:\mathrm{Va}}\right)\Big/3\\
&\cong \left[\Delta G^{\alpha}_{MN}(x_{\mathrm{Fe}}, x_{X_1}, 0, \cdots) - \Delta G^{\alpha}_{MN}(1,0,0,\cdots)\right]\\
&\quad + \left[\Delta G^{\alpha}_{MN}(x_{\mathrm{Fe}}, 0, x_{X_2}, \cdots) - \Delta G^{\alpha}_{MN}(1,0,0,\cdots)\right]\\
&\quad + \cdots - \left(\sum_i x_{X_i}\sum_i x_{X_i} - \sum_i x_{X_i}x_{X_i}\right)L^{\mathrm{bcc}}_{\mathrm{Fe},X_1:\mathrm{Va}}\\
&\quad + \left(\sum_i x_{X_i}\sum_i x_{X_i} - \sum_i x_{X_i}x_{X_i}\right)\\
&\quad \times \left(L^{\mathrm{bcc}}_{\mathrm{Fe},X_1:N} - L^{\mathrm{bcc}}_{\mathrm{Fe},X_1:\mathrm{Va}}\right)\Big/3 \cong G^{\alpha}_{MN}(x_{\mathrm{Fe}}, x_{X_1}, 0, \cdots)\\
&\quad - \Delta G^{\alpha}_{MN}(1,0,0,\cdots) + \Delta G^{\alpha}_{MN}(x_{\mathrm{Fe}}, 0, x_{X_2}, \cdots)\\
&\quad - \Delta G^{\alpha}_{MN}(1,0,0,\cdots) + \cdots
\end{aligned} \quad [A3b]$$

$$\begin{aligned}
&\log\frac{A^2_{\mathrm{Fe}}}{\left[A_{\mathrm{Fe}}\left(1-\sum_i x_{X_i}\right) + \sum_i x_{X_i}A_{X_i}\right]^2}\\
&= \log\frac{A^2_{\mathrm{Fe}}}{\left[A_{\mathrm{Fe}}\left(1-x_{X_1}\right) + x_{X_1}A_{X_1}\right]^2}\\
&\quad + \log\frac{A^2_{\mathrm{Fe}}}{\left[A_{\mathrm{Fe}}\left(1-x_{X_2}\right) + x_{X_2}A_{X_2}\right]^2} + \cdots\\
&\quad + \log\frac{\prod_i\left[A_{\mathrm{Fe}}\left(1-x_{X_1}\right) + x_{X_1}A_{X_1}\right]^2}{A^{2i-2}_{\mathrm{Fe}}\left[A_{\mathrm{Fe}}\left(1-\sum_i x_{X_i}\right) + \sum_i x_{X_i}A_{X_i}\right]^2}\\
&\cong \log\frac{A^2_{\mathrm{Fe}}}{\left[A_{\mathrm{Fe}}\left(1-x_{X_1}\right) + x_{X_1}A_{X_1}\right]^2}\\
&\quad + \log\frac{A^2_{\mathrm{Fe}}}{\left[A_{\mathrm{Fe}}\left(1-x_{X_2}\right) + x_{X_2}A_{X_2}\right]^2} + \cdots
\end{aligned} \quad [A3c]$$

By substituting Eqs. [A3b] and [A3c] into Eq. [A3a], Eq. [13] is deduced.

NOMENCLATURE

$X_i, X_{i'}$	i-th and i'-th ($i' < i$) solid solution elements (not compound formed elements) in ferrite, of which atoms fill in the first sublattice
M	Binary compound formed element, of which atoms fill in the first sublattice
N	Binary compound formed element, of which atoms fill in the second sublattice
Va	Vacancy, which fills in the second sublattice
G^{α}	Gibbs energy of α phase (J/mol)
${}^{mg}G^{a}$	Magnetic contribution to Gibbs energy, which is proposed by Inden[5] and modified by Hillert and Jarl[6] (J/mol)
G^{P}	Gibbs energy of binary compound
j, j'	Element types in first sublattice (in the order of Fe, X_1, X_2, … and M; the sequence number of j' is smaller than that of j)
k, k'	Element types in second sublattice (in the order of N and Va; the sequence number of k' is smaller than that of k)
${}^{\circ}G^{\mathrm{bcc}}_{j:k}$	Gibbs energy of body-centered-cubic (bcc) phase where the first and second sublattices are filled with j atoms and k atoms, respectively (J/mol)
${}^{\circ}G^{\mathrm{fcc}}_{j:k}$	Gibbs energy of face-centered-cubic (fcc) phase where the first and second sublattices are filled with j atoms and k atoms, respectively (J/mol)
$\mu^{\mathrm{bcc}}_{j:k}$	Chemical potential of bcc phase where the first and second sublattices are filled with j atoms and k atoms, respectively (J/mol)
μ^{bcc}_{j}	Chemical potential of j element in bcc phase
μ^{bcc}_{k}	Chemical potential of k element in bcc phase
$\mu^{\mathrm{fcc}}_{j:k}$	Chemical potential of fcc binary compound where the first and second sublattices are filled with j atoms and k atoms, respectively (J/mol)
L^{bcc}	Interaction parameter of bcc phase (in the subscripts of L^{bcc}, components in different sublattices are separated by a colon and, in the same sublattice, by a comma) (J/mol)
β^{bcc}	Quantity related to total magnetic entropy of bcc phase
T^{bcc}_{c}	Critical temperature for magnetic ordering of bcc phase
${}^{0}T^{\mathrm{bcc}}_{cj}$	Magnetic interaction parameter of pure j atoms in bcc phase related to critical temperature for magnetic ordering (Kelvin)
${}^{0}\beta^{\mathrm{bcc}}_{j}$	Magnetic parameter of pure j atoms in bcc phase related to magnetic entropy
${}^{n}T^{\mathrm{bcc}}_{cj,j'}$	The n-th binary magnetic interaction parameter between j atoms and j' atoms in bcc phase related to critical temperature for magnetic ordering (Kelvin)
${}^{n}\beta^{\mathrm{bcc}}_{j,j'}$	The n-th binary magnetic interaction parameter between j atoms and j' atoms in bcc phase related to magnetic entropy
y^{α}_{j}	Site fraction of j atoms in the first sublattice in ferrite
y^{α}_{k}	Site fraction of k atoms in the second sublattice in ferrite
$f(\tau)$	Polynomial function, which is obtained by Hillert and Jarl[6] based on the magnetic specific heat of iron
T	Temperature (K)
R	Universal gas constant (J/mol K)
τ	Ratio of T to T^{bcc}_{c}
p	Ratio of magnetic enthalpy due to short-ordering to the total amount of magnetic enthalpy, $p = 0.4$ for bcc structure[6]
x_m	Mole fraction of m element in the system
[wt pct m]	Mass percent of m element in ferrite
A_m	Relative atomic mass of m element
$\log^{\alpha}K^{0}_{MN}$	Logarithmic solubility product of binary compound MN in pure ferrite in the Fe-M-N system
$\log^{\alpha}K^{X_i}_{MN}$	Logarithmic solubility product of binary compound MN in ferrite in the Fe-X_i-M-N system
$\Delta\log^{\alpha}K^{X_i}_{MN}$	Increment of logarithmic solubility product of binary compound MN in ferrite for solid solution element X_i addition
$\log^{\alpha}K_{MN}$	Logarithmic solubility product of binary compound MN in ferrite in the Fe-X_1-X_2-… M-N system

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