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Journal of Alloys and Compounds 321 (2001) 242–247

Journal of ALLOYS AND COMPOUNDS

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Enthalpies of mixing in Fe–C–Si melts

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Received 5 September 2000; accepted 5 December 2000

Abstract

The enthalpy of mixing of molten Fe–C–Si alloys is a significant element in performing mass balances on iron production and steelmaking, but almost no experimental data has been reported on enthalpy determination in these melts. As a result, models expressing this property as a function of composition must be derived from measurements of component activity, which are more widely available. The use of three such models – the regular solution model, Wagner's model for dilute solutions, and the unified interaction parameter model developed by Bale and Pelton – have been used to calculate enthalpies of mixing in Fe–C–Si melts. The results are compared with each other and with the experimental data of Vitusevich et al. © 2001 Elsevier Science B.V. All rights reserved.

Keywords: Enthalpy of mixing; Ternary melts; Fe–C–Si

1. Introduction

In performing energy balances on furnaces processing liquid iron alloys, one of the less-appreciated but significant factors is the enthalpy of mixing of the alloy. This is particularly true in the case of iron–carbon–silicon alloys, which are produced in the blast furnace as hot metal and in the cupola as cast iron, and converted to steel by oxidation of the dissolved carbon and silicon during the BOF process. Healy and McBride [1] have shown that about 3% of the enthalpy input to hot metal conversion is obtained from the 'unmixing' of liquid pig iron to the constituent elements, while Fine and Geiger [2] have demonstrated that the enthalpies of carbon and silicon oxidation are changed by +5% and −14%, respectively, when the enthalpy of mixing is considered. Others [3–5] have taken into account alloy enthalpies of mixing in constructing energy balances for blast-furnace operation.

However, including enthalpies of mixing into energy-balance calculations involving molten hot metal or cast iron has always been made difficult by the lack of experimental data for the system. Carbon dissolves slowly in molten iron alloys, and as a result no direct experimental measurements of ΔH_{mix} for carbon have been determined even in binary Fe–C melts [6,7]. The only known measurements for the ternary Fe–C–Si system are those of Vitusevich et al. [6–8], who determined the partial enthalpy of mixing of silicon in Fe–Si and Fe–C–Si melts at 1587°C. A map showing modeled partial enthalpies of mixing was determined from these results, based on a limited number of ternary-system data points.

Given the lack of experimental data on enthalpies of mixing in Fe–C–Si melts, the construction of energy balances involving these alloys has instead relied on dubious assumptions. One common assumption [2–5,9] is that the enthalpies of mixing of carbon and silicon in ternary alloys are equal to the infinite-dilution enthalpy of mixing of these elements in binary Fe–C and Fe–Si melts [10]. This approach carries two inherent sources of inaccuracy. The first is that hot metal is generally not a dilute solution, especially with regard to carbon, and the enthalpy of mixing may be highly dependent on concentration, as Healy and McBride point out [1]. The second difficulty with using infinite-dilution enthalpies of mixing is that this approach ignores the potential impact of ternary-system interactions on this property. As a result, an improved approach for estimating enthalpies of mixing in Fe–C–Si melts is needed.

While very little experimental work has been performed on the measurements of enthalpies of mixing in molten Fe–C–Si, a much more extensive experimental database is available for Gibbs energy-related thermodynamic properties, in particular the activities of carbon and silicon. As a result, it is possible to develop estimated enthalpies of mixing by modeling the activity data. This presentation

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PII: S0925-8388(01)00959-8

will examine several methods of such modeling, and compare the resulting ΔH_{mix} values with those from different models and the existing experimental work [6–8].

2. The regular-solution model

One previous effort has been made to use phase-equilibria data to model enthalpies of solution in molten Fe–C–Si alloys. Schmid's work [11] relies on a four-suffix regular-solution model in which the excess Gibbs energy of mixing for a multicomponent solution can be represented by:

$$\Delta G^{\mathrm{E}} = \sum_{i,j,k,l} a_{ijkl} X_i X_j X_k X_l \tag{1}$$

Application of the Gibbs-Duhem relationship converts this to an expression for the activity coefficient of component r:

$$RT \ln\gamma_r = 4 \sum_{i,j,k} a_{ijkr} X_i X_j X_k - 3 \sum_{i,j,k,l} a_{ijkl} X_i X_j X_k X_l \tag{2}$$

The a values are in turn a linear function of temperature, e.g.

$$a_{ijkl} = h_{ijkl} - Ts_{ijkl} \tag{3}$$

Eq. (3) implies that the enthalpy and entropy of mixing in molten Fe–C–Si alloys is independent of temperature, at least over short ranges. As a result, the partial enthalpy of mixing can be written in a fashion similar to Eq. (2):

$$\Delta \bar{H}_r = 4 \sum_{i,j,k} h_{ijkr} X_i X_j X_k - 3 \sum_{i,j,k,l} h_{ijkl} X_i X_j X_k X_l \tag{4}$$

Expanding this expression for the Fe–C–Si system generates expressions for the partial enthalpies of mixing of Fe, C and Si:

$$\begin{aligned}
\Delta \bar{H}_{\mathrm{C}} = &\left(12X_{\mathrm{C}}^2 X_{\mathrm{Si}} - 12X_{\mathrm{C}}^3 X_{\mathrm{Si}}\right) h_{\mathrm{CCCSi}} \\
&+\left(12X_{\mathrm{C}} X_{\mathrm{Si}}^3 - 18X_{\mathrm{C}}^2 X_{\mathrm{Si}}^2\right) h_{\mathrm{CCSiSi}} \\
&+\left(4X_{\mathrm{Si}}^3 - 12X_{\mathrm{C}} X_{\mathrm{Si}}^3\right) h_{\mathrm{CSiSiSi}} \\
&+\left(12X_{\mathrm{Fe}} X_{\mathrm{C}}^2 - 12X_{\mathrm{Fe}} X_{\mathrm{C}}^3\right) h_{\mathrm{FeCCC}} \\
&+\left(12X_{\mathrm{Fe}}^2 X_{\mathrm{C}} - 18X_{\mathrm{Fe}}^2 X_{\mathrm{C}}^2\right) h_{\mathrm{FeFeCC}} \\
&+\left(4X_{\mathrm{Fe}}^3 - 12X_{\mathrm{Fe}}^3 X_{\mathrm{C}}\right) h_{\mathrm{FeFeFeC}} \\
&- 12X_{\mathrm{Fe}}^3 X_{\mathrm{Si}} h_{\mathrm{FeFeFeSi}} - 18X_{\mathrm{Fe}}^2 X_{\mathrm{Si}}^2 h_{\mathrm{FeFeSiSi}} \\
&- 12X_{\mathrm{Fe}} X_{\mathrm{Si}}^3 h_{\mathrm{FeSiSiSi}} \\
&+\left(12X_{\mathrm{Fe}}^2 X_{\mathrm{Si}} - 36X_{\mathrm{Fe}}^2 X_{\mathrm{C}} X_{\mathrm{Si}}\right) h_{\mathrm{FeFeCSi}} \\
&+\left(12X_{\mathrm{Fe}} X_{\mathrm{Si}}^2 - 36X_{\mathrm{Fe}} X_{\mathrm{C}} X_{\mathrm{Si}}^2\right) h_{\mathrm{FeCSiSi}} \\
&+\left(24X_{\mathrm{Fe}} X_{\mathrm{C}} X_{\mathrm{Si}} - 36X_{\mathrm{Fe}} X_{\mathrm{C}}^2 X_{\mathrm{Si}}\right) h_{\mathrm{FeCCSi}}
\end{aligned} \tag{5}$$

$$\begin{aligned}
\Delta \bar{H}_{\mathrm{Si}} = &\left(12X_{\mathrm{Si}}^2 X_{\mathrm{Fe}} - 12X_{\mathrm{C}}^3 X_{\mathrm{Fe}}\right) h_{\mathrm{SiSiSiFe}} \\
&+\left(12X_{\mathrm{Si}} X_{\mathrm{Fe}}^3 - 18X_{\mathrm{Si}}^2 X_{\mathrm{Fe}}^2\right) h_{\mathrm{SiSiFeFe}} \\
&+\left(4X_{\mathrm{Fe}}^3 - 12X_{\mathrm{Si}} X_{\mathrm{Fe}}^3\right) h_{\mathrm{SiFeFeFe}} \\
&+\left(12X_{\mathrm{C}} X_{\mathrm{Si}}^2 - 12X_{\mathrm{C}} X_{\mathrm{Si}}^3\right) h_{\mathrm{CSiSiSi}} \\
&+\left(12X_{\mathrm{C}}^2 X_{\mathrm{Si}} - 18X_{\mathrm{C}}^2 X_{\mathrm{Si}}^2\right) h_{\mathrm{CCSiSi}} \\
&+\left(4X_{\mathrm{C}}^3 - 12X_{\mathrm{C}}^3 X_{\mathrm{Si}}\right) h_{\mathrm{CCCSi}} \\
&- 12X_{\mathrm{C}}^3 X_{\mathrm{Fe}} h_{\mathrm{CCCFe}} - 18X_{\mathrm{C}}^2 X_{\mathrm{Fe}}^2 h_{\mathrm{CCFeFe}} \\
&- 12X_{\mathrm{CX_{Fe}^3}} h_{\mathrm{CFeFeFe}} \\
&+\left(12X_{\mathrm{C}}^2 X_{\mathrm{Fe}} - 36X_{\mathrm{C}}^2 X_{\mathrm{Si}} X_{\mathrm{Fe}}\right) h_{\mathrm{CCSiFe}} \\
&+\left(12X_{\mathrm{C}} X_{\mathrm{Fe}}^2 - 36X_{\mathrm{C}} X_{\mathrm{Si}} X_{\mathrm{Fe}}^2\right) h_{\mathrm{CSiFeFe}} \\
&+\left(24X_{\mathrm{Fe}} X_{\mathrm{C}} X_{\mathrm{Si}} - 36X_{\mathrm{Fe}} X_{\mathrm{C}}^2 X_{\mathrm{Si}}\right) h_{\mathrm{FeCCSi}}
\end{aligned} \tag{6}$$

$$\begin{aligned}
\Delta \bar{H}_{\mathrm{Fe}} = &\left(12X_{\mathrm{Fe}}^2 X_{\mathrm{C}} - 12X_{\mathrm{Fe}}^3 X_{\mathrm{C}}\right) h_{\mathrm{FeFeFeC}} \\
&+\left(12X_{\mathrm{Fe}} X_{\mathrm{C}}^3 - 18X_{\mathrm{Fe}}^2 X_{\mathrm{C}}^2\right) h_{\mathrm{FeFeCC}} \\
&+ \left(4X_{\mathrm{C}}^3 - 12X_{\mathrm{Fe}} X_{\mathrm{C}}^3\right) h_{\mathrm{FeCCC}} \\
&+\left(12X_{\mathrm{Si}} X_{\mathrm{Fe}}^2 - 12X_{\mathrm{Si}} X_{\mathrm{Fe}}^3\right) h_{\mathrm{SiFeFeFe}} \\
&+\left(12X_{\mathrm{Si}}^2 X_{\mathrm{Fe}} - 18X_{\mathrm{Si}}^2 X_{\mathrm{Fe}}^2\right) h_{\mathrm{SiSiFeFe}} \\
&+\left(4X_{\mathrm{Si}}^3 - 12X_{\mathrm{Si}}^3 X_{\mathrm{Fe}}\right) h_{\mathrm{SiSiSiFe}} - 12X_{\mathrm{Si}}^3 X_{\mathrm{C}} h_{\mathrm{SiSiSiC}} \\
&- 18X_{\mathrm{Si}}^2 X_{\mathrm{C}}^2 h_{\mathrm{SiSiCC}} - 12X_{\mathrm{Si}} X_{\mathrm{C}}^3 h_{\mathrm{SiCCC}} \\
&+\left(12X_{\mathrm{Si}}^2 X_{\mathrm{C}} - 36X_{\mathrm{Si}}^2 X_{\mathrm{Fe}} X_{\mathrm{C}}\right) h_{\mathrm{SiSiFeC}} \\
&+\left(12X_{\mathrm{Si}} X_{\mathrm{C}}^2 - 36X_{\mathrm{Si}} X_{\mathrm{Fe}} X_{\mathrm{C}}^2\right) h_{\mathrm{SiFeCC}} \\
&+\left(24X_{\mathrm{Fe}} X_{\mathrm{C}} X_{\mathrm{Si}} - 36X_{\mathrm{Fe}} X_{\mathrm{C}}^2 X_{\mathrm{Si}}\right) h_{\mathrm{FeCCSi}}
\end{aligned} \tag{7}$$

Parameters featuring only two of the components (e.g. h_{FeFeSiSi}) can be determined from analysis of the appropriate binary system. The number of variables to be determined is simplified by 'cyclic permutation,' such that if iron is element 1, C is element 2, and Si is element 3, $h_{\mathrm{FeSiCC}} = h_{\mathrm{CFeSiSi}} = h_{\mathrm{SiCFeFe}}$. Furthermore, all the ternary-system parameters are equal, so that a total of only 10 variables is needed to use the model.

As previously mentioned, very little experimental data exists for enthalpies of mixing in Fe–C–Si melts. However, a substantial number of investigators have determined the activities (and thus the activity coefficients) of dissolved C and/or Si in these solutions, as a function of both temperature and composition. This allows the determination by regression analysis of a_{ijkl} for different compositions as a function of temperature; the function of temperature in turn determines h_{ijkl} and s_{ijkl}. Table 1 illustrates the values of h_{ijkl} in the Fe–C–Si system determined by Schmid [11]; by inserting these into Eqs. (4)–(7), partial enthalpies of mixing with respect to liquid iron and silicon and solid carbon can be calculated. The total enthalpy of mixing can be calculated by,

$$\Delta H_{\mathrm{mix}} = \Delta \bar{H}_{\mathrm{Fe}} X_{\mathrm{Fe}} + \Delta \bar{H}_{\mathrm{C}} X_{\mathrm{C}} + \Delta \bar{H}_{\mathrm{Si}} X_{\mathrm{Si}} \tag{8}$$

Table 1
Parameters for the regular-solution model for Fe–C–Si melts (after Schmid [11])

	h_{ijkl} (J/g-atom)
Binary-system parameters	
h_{FeFeFeC}	−38 806
h_{FeFeCC}	−87 103
h_{FeCCC}	−29 916
h_{FeFeFeSi}	−33 633
h_{FeFeSiSi}	−68 923
h_{FeSiSiSi}	−26 190
h_{CCCSi}	327 070
h_{CCSiSi}	436 090
h_{CSiSiSi}	327 070
Ternary-system parameter	
$h_{\mathrm{FeFeCSi}} = h_{\mathrm{CCSiFe}} = h_{\mathrm{SiSiFeC}} =$ $h_{\mathrm{FeCCSi}} = h_{\mathrm{CSiSiFe}} = h_{\mathrm{SiFeFeC}} =$ $h_{\mathrm{FeCSiSi}} h_{\mathrm{CSiFeFe}} = h_{\mathrm{SiFeCC}}$	−81 071

Using these values and Eqs. (4)–(8), values of ΔH_{mix} have been calculated for Fe–C–Si alloys as a function of composition. These are shown mapped in Fig. 1. As expected, they become more negative as the silicon content increases, and somewhat surprisingly more negative with increasing carbon content as well.

3. The dilute-solution model

A simpler model for calculating thermodynamic properties in relatively dilute solutions stems from the work of Wagner [12]. Wagner's model states that the activity coefficient of solutes in melts such as these can be expressed at a given temperature as a function of composition:

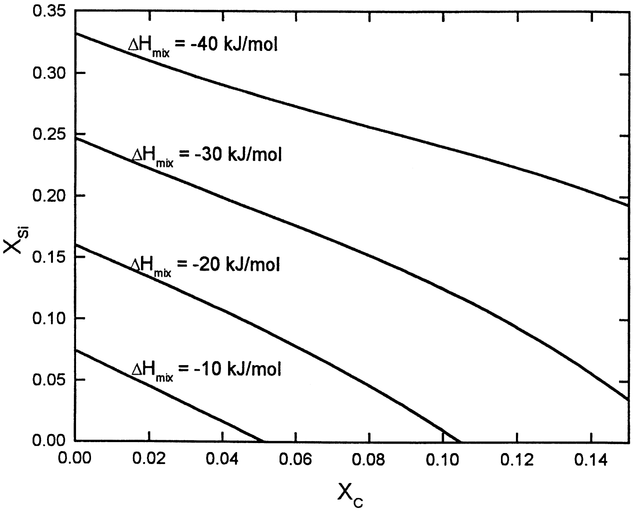

Fig. 1. Predicted enthalpies of mixing of Fe–C–Si melts calculated using the regular-solution model [11].

$$\ln \gamma_r = \ln \gamma_r^o + \sum_i \varepsilon_r^i X_i \tag{9}$$

where ε_r^i is the first-order interaction parameter for solute i on solute r, and γ_r^o is the infinite-dilution activity coefficient of r in the solvent metal. ln γ_r^o and ε_r^i are linear functions of inverse temperature:

$$\ln \gamma_r^o = A/T + B \tag{10}$$

$$\varepsilon_r^i = C/T + D \tag{11}$$

As a result, ln γ_r can be determined as a function of composition and temperature. The derivative of ln γ_r with respect to inverse temperature is proportional to the partial enthalpy of mixing:

$$\frac{\partial \ln \gamma_r}{\partial (1/T)} = \frac{\Delta \bar{H}_r}{R} \tag{12}$$

The model assumes that the activity of the solvent metal (in this case iron) is equal to one, thereby making its partial enthalpy of mixing equal to zero. Eq. (9) can be extended by the use of a second-order interaction parameter, but the uncertainty level of the experimental data from which interaction parameters are obtained is such that this is rarely justified.

Sigworth and Elliott [13] have compiled equations for most of the parameters needed to apply Wagner's model to the Fe–C–Si system:

$$\ln \gamma_{\mathrm{C}}^o = -2.013 + 2717/T \tag{13}$$

$$\varepsilon_{\mathrm{C}}^{\mathrm{C}} = 3.55 + 7830/T \tag{14}$$

$$\varepsilon_{\mathrm{C}}^{\mathrm{Si}} = \varepsilon_{\mathrm{Si}}^{\mathrm{C}} = -0.4294 + 18\,760/T \tag{15}$$

Other needed parameters can be obtained from the work of Dresler [14]:

$$\ln \gamma_{\mathrm{Si}}^o = 2.93 - 17\,014/T \tag{16}$$

$$\varepsilon_{\mathrm{Si}}^{\mathrm{Si}} = 7.039 + 7898/T \tag{17}$$

From these, the partial enthalpies of mixing of carbon and silicon can be determined as a function of composition:

$$\Delta \bar{H}_{\mathrm{C}} = 22\,590 + 65\,102 X_{\mathrm{C}} + 155\,978 X_{\mathrm{Si}} \tag{18}$$

$$\Delta \bar{H}_{\mathrm{Si}} = -141\,461 + 156\,003 X_{\mathrm{C}} + 65\,667 X_{\mathrm{Si}} \tag{19}$$

Fig. 2 shows the resulting enthalpies of mixing for Fe–C–Si melts, plotted in the same fashion as Fig. 1. The values are considerably less negative than those calculated using the regular-solution model, especially at higher carbon contents; in addition, the influence of carbon content is less pronounced than that seen in Fig. 1.

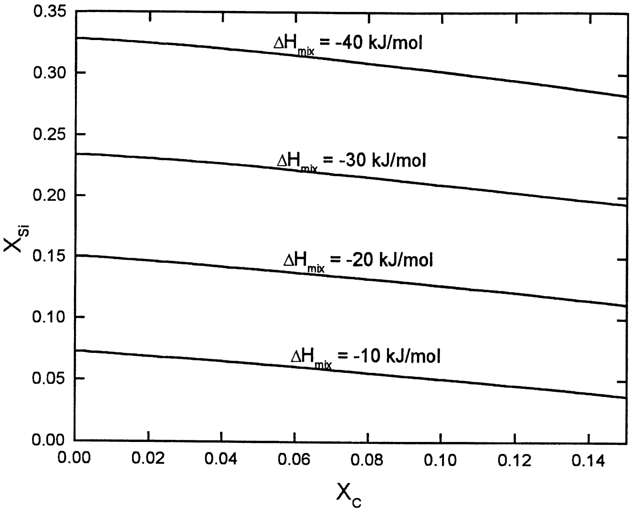

Fig. 2. Predicted enthalpies of mixing of Fe–C–Si melts calculated using the dilute-solution model of Wagner [12].

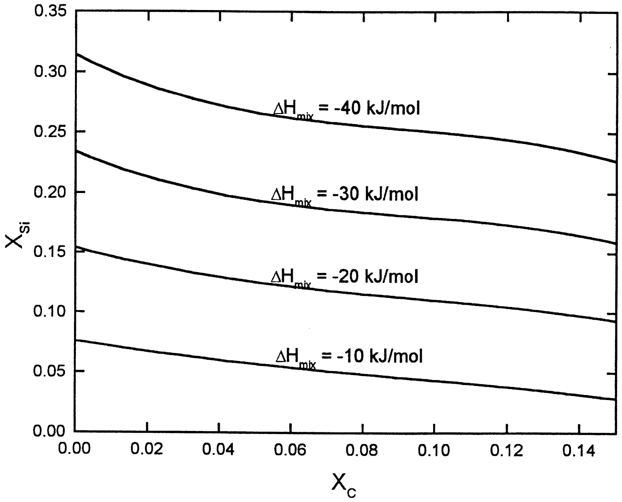

Fig. 3. Predicted enthalpies of mixing of Fe–C–Si melts calculated using the unified interaction-parameter model of Pelton and Bale [15].

4. The unified interaction parameter model

One of the difficulties in using Wagner's model for calculating solute activities is its primary applicability to dilute solutions. As solute concentrations grow, the model increasingly requires the use of a second-order interaction parameter to accurately reflect the relationship between ln γ_r and X_r; since these are rarely available, the reliability of calculations made using this approach becomes more suspect. The increasingly reduced activity of the solvent also makes it difficult to support the notion that its partial Gibbs energy of mixing (and thus its enthalpy of mixing) is equal to zero.

Bale and Pelton have derived a revised version of Wagner's model consistent with the Gibbs-Duhem expression, and more appropriate for non-dilute solutions [15]. Their approach relies on a 'unified interaction parameter' similar to the interaction parameter described by Wagner [12]. For a first-order relationship,

$$\ln \gamma_r = \ln \gamma_r^o + \ln \gamma_{\text{solvent}} + \sum_{j=1}^{N} \varepsilon_{rj} X_j \qquad (20)$$

The activity coefficient of the solvent is determined by,

$$\ln \gamma_{\text{solvent}} = -\frac{1}{2} \sum_{j,k=1}^{N} \varepsilon_{jk} X_j X_k \qquad (21)$$

As the mole fraction of solvent approaches unity, ln γ_{solvent} approaches zero, making the value of the unified interaction parameter ε_{jk} equal to the Wagner interaction parameter ε_k^j. As a result, Eqs. (13)–(17) can be used for calculating these values as well. The difference between the two models is the non-zero value of ln γ_{solvent} in non-dilute solutions. This makes the partial enthalpy of mixing of the solvent a non-zero value as well.

Using this approach, enthalpies of mixing have been calculated as a function of composition and are again mapped in Fig. 3. As might be suspected, the results are similar to those of Fig. 2 at low alloy content, diverging slightly as the carbon and silicon contents decrease. The revised model tends to generate slightly less exothermic enthalpies of mixing as the divergence becomes noticeable.

5. Comparison of models

Figs. 4 and 5 illustrate the calculated enthalpies of mixing in iron–carbon–silicon melts as a function of composition, using the different models. At the low carbon concentration ($X_C = 0.01$) shown in Fig. 4, the three models produce little difference in ΔH_{mix}; however, as the carbon content grows in Fig. 5 ($X_C = 0.10$), the values predicted by

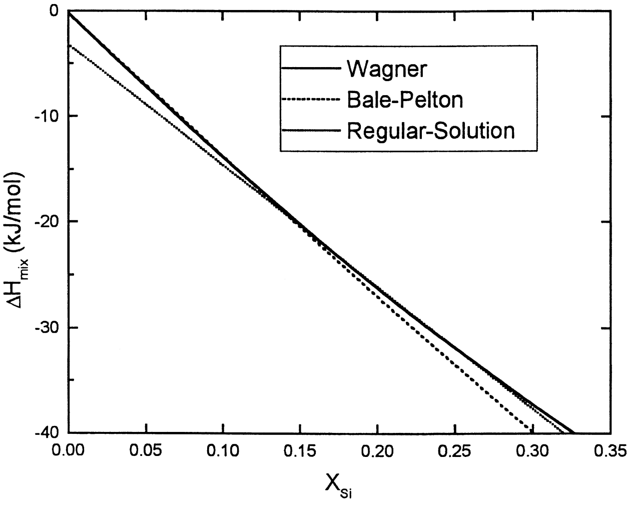

Fig. 4. Predicted enthalpies of mixing of Fe–C–Si melts calculated using the three models, at constant $X_C = 0.01$.

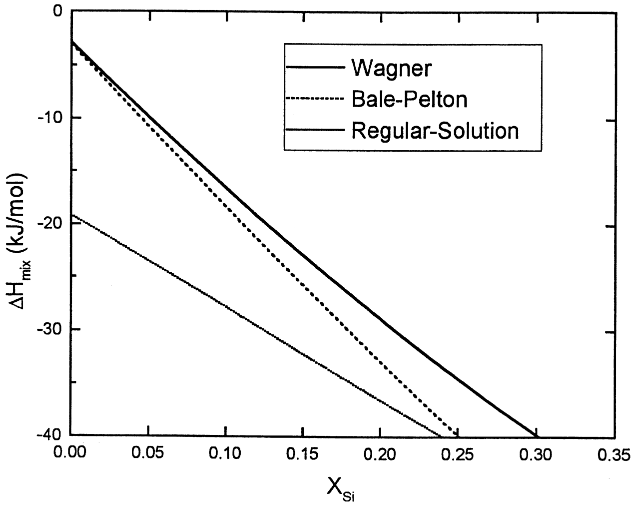

Fig. 5. Predicted enthalpies of mixing of Fe–C–Si melts calculated using the three models, at constant $X_C = 0.10$.

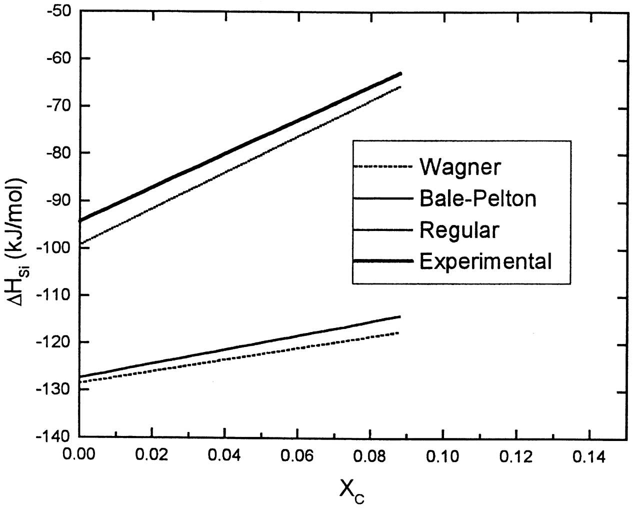

Fig. 7. Predicted partial molar enthalpies of mixing of silicon in Fe–C–Si melts ($X_{Si} = 0.25$) calculated using the three models, compared with results obtained from the experimental work of Vitusevich et al. [7].

the regular-solution model diverge noticeably from those of the other two. The impact of added carbon content on the enthalpy of mixing at constant silicon levels makes it clear that the use of separate elemental enthalpies of mixing, as practiced in previous mass-balance calculations [2–5,9], leaves something to be desired in terms of accuracy.

As previously mentioned, some experimental measurements have been made in the system by Vitusevich et al. [6,7], and these provide a basis for assessing the accuracy of the models. Fig. 6 compares enthalpies of mixing predicted by the three models at $X_{Si} = 0.05$ and varying carbon content with the experimentally-derived function of composition; Fig. 7 shows a similar comparison at $X_{Si} = 0.25$. The level of agreement is not especially impressive, although the regular-solution clearly matches the experimental data better in highly alloyed compositions. Again, the impact of solute interactions on the calculated partial enthalpies of mixing is apparent in both the experimental and modeled values.

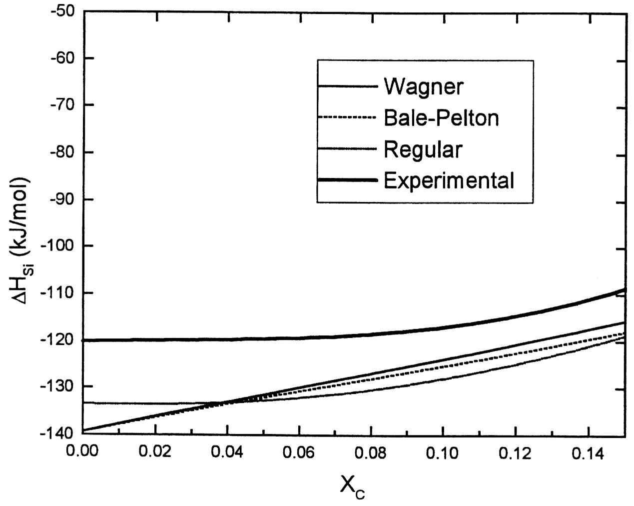

Fig. 6. Predicted partial molar enthalpies of mixing of silicon in Fe–C–Si melts ($X_{Si} = 0.05$) calculated using the three models, compared with results obtained from the experimental work of Vitusevich et al. [7].

6. Conclusions

At relatively low concentrations of carbon and silicon, any of these three models will generate reasonably reliable estimated enthalpies of mixing in Fe–C–Si melts. The models are all adaptable to more complex melts (e.g. Fe–Mn–Si–C–P–S, etc.), although the needed data for this are more available if the Wagner and Bale-Pelton models are used. At very high alloy concentrations, the regular-solution model may yield more accurate results, although the occurrence of these alloys in practice is rare. Further studies of these three (and possibly other) models in systems with more experimental enthalpy-of-mixing data to compare with would be of more than some interest.

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