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Prediction of the thermodynamic properties of solutes in Pb-based dilute solutions

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Abstract

The coordination numbers in the Molecular Interaction Volume Model (MIVM) can be calculated from common physical quantities for pure metals. A significant advantage of the model lies in its ability to predict thermodynamic properties of solutes in Pb-based dilute solutions using only binary infinite dilute activity coefficients, and the predicted values are in good agreement with the experimental data for Pb-based dilute solutions. This shows that the model is reliable, convenient and economic. © 2002 Elsevier Science B.V. All rights reserved.

Keywords: Thermodynamic properties; The Pb-based dilute solutions; Molecular interaction volume model; Modified coordination equation

1. Introduction

The thermodynamic properties of multicomponent liquid alloys are important for understanding process metallurgy and the metal alloying. A great deal of binary data has so far been compiled in monographs such as Hultgren et al. [1], but multicomponent data is scattered in journals and is quite scarce because the determination of thermodynamic data of multicomponent systems not only needs the consummate skill of research workers, but also excellent instrument and continuous financial support. Furthermore, numerous multicomponent systems are common in industrial processes. It is obviously unrealistic to obtain all the data experimentally. Therefore, a unique economic and effective method to predict the behaviors of multicomponent systems by theory or by thermodynamic models depending on less experimental data is required.

The interaction parameter formalism first proposed by Wagner [2] is frequently used to represent the thermodynamic properties of dilute solutions, particularly for iron-based alloys. Furthermore, the formalism is often used to compute activity coefficients at solute concentrations of several atomic percent. Depending upon the system, at these concentrations, the thermodynamic inconsistency can result in significant errors [3]. On the other hand, the formalism is mathematically exact if the Maclaurin series for the logarithm of the activity coefficient of a solute in a multicomponent system is not truncated as in the treatment of Lupis and Elliott [4]. However, higher order interaction parameters are rarely available for systems of practical interest. Moreover, the measurement of the interacton coefficients beyond second order requires accuracies of measurement which are difficult to obtain in practice. It is, therefore, often necessary to calculate activity coefficients of solutes at finite concentrations using only the first or second-order interaction parameters [5]. Although, as dis-

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cussed by Darken [6], the formalism is limited to infinite dilution and is thermodynamically inconsistent at finite concentrations, this point of theory is still the subject of debate [3,5,7,8]. The purpose of this work is to show that the Molecular Interaction Volume Model (MIVM) proposed by the Tao [9] can predict the thermodynamic properties of solutes in the Pb-based dilute solutions using only the corresponding binary infinite dilute activity coefficients and the coordination numbers of the constituent elements in liquid alloys.

2. Molecular interaction volume model [9]

The MIVM was obtained in the physical sense of liquid molecular movements in that liquid molecules are not like gas molecules which are in continuous irregular motion and not like solid ones which are vibrating constantly at one site but are migrating nonrandomly from one cell to another. The molar excess Gibbs energy $G_{\mathrm{m}}^{\mathrm{E}}$ of the liquid mixture $i-j$

$$\frac{G_{\mathrm{m}}^{\mathrm{E}}}{RT} = x_i \ln\left(\frac{V_{\mathrm{m}i}}{x_iV_{\mathrm{m}i} + x_jV_{\mathrm{m}j}B_{ji}}\right) + x_j \ln\left(\frac{V_{\mathrm{m}j}}{x_jV_{\mathrm{m}j} + x_iV_{\mathrm{m}i}B_{ij}}\right) - \frac{x_ix_j}{2} \times \left(\frac{Z_iB_{ji}\ln B_{ji}}{x_i + x_jB_{ji}} + \frac{Z_jB_{ij}\ln B_{ij}}{x_j + x_iB_{ij}}\right) \quad (1)$$

as well as the new expressions of activity coefficients of the components i and j, respectively

$$\ln\gamma_i = \ln\left(\frac{V_{\mathrm{m}i}}{x_iV_{\mathrm{m}i} + x_jV_{\mathrm{m}j}B_{ji}}\right) + x_j\left(\frac{V_{\mathrm{m}j}B_{ji}}{x_iV_{\mathrm{m}i} + x_jV_{\mathrm{m}j}B_{ji}} - \frac{V_{\mathrm{m}i}B_{ij}}{x_jV_{\mathrm{m}j} + x_iV_{\mathrm{m}i}B_{ij}}\right) - \frac{x_j^2}{2}\left(\frac{Z_iB_{ji}^2\ln B_{ji}}{(x_i + x_jB_{ji})^2} + \frac{Z_jB_{ij}\ln B_{ij}}{(x_j + x_iB_{ij})^2}\right) \quad (2)$$

$$\ln\gamma_j = \ln\left(\frac{V_{\mathrm{m}j}}{x_jV_{\mathrm{m}j} + x_iV_{\mathrm{m}i}B_{ij}}\right) - x_i\left(\frac{V_{\mathrm{m}j}B_{ji}}{x_iV_{\mathrm{m}i} + x_jV_{\mathrm{m}j}B_{ji}} - \frac{V_{\mathrm{m}i}B_{ij}}{x_jV_{\mathrm{m}j} + x_iV_{\mathrm{m}i}B_{ij}}\right) - \frac{x_i^2}{2}\left(\frac{Z_iB_{ij}^2\ln B_{ij}}{(x_j + x_iB_{ij})^2} + \frac{Z_iB_{ji}\ln B_{ji}}{(x_i + x_jB_{ji})^2}\right) \quad (3)$$

Extending Eq. (1) to a multicomponent mixture, its molar excess Gibbs energy can be generalized as

$$\frac{G_{\mathrm{m}}^{\mathrm{E}}}{RT} = \sum_{i=1}^{n} x_i \ln\frac{V_{\mathrm{m}i}}{\sum_{j=1}^{n} x_jV_{\mathrm{m}j}B_{ji}} - \frac{1}{2}\sum_{i=1}^{n} Z_ix_i\left(\frac{\sum_{j=1}^{n} x_jB_{ji}\ln B_{ji}}{\sum_{k=1}^{n} x_kB_{ki}}\right) \quad (4)$$

and the expression of activity coefficient of any component i is

$$\ln\gamma_i = 1 + \ln\frac{V_{\mathrm{m}i}}{\sum_{j=1}^{n} x_jV_{\mathrm{m}j}B_{ji}} - \sum_{t=1}^{n}\frac{x_kV_{\mathrm{m}i}B_{ik}}{\sum_{j=1}^{n} x_jV_{\mathrm{m}j}B_{jk}} - \frac{1}{2}\left(\frac{Z_i\sum_{j=1}^{n} x_jB_{ji}\ln B_{ji}}{\sum_{l=1}^{n} x_lB_{li}} + \sum_{j=1}^{n}\frac{Z_jx_jB_{ij}}{\sum_{l=1}^{n} x_lB_{lj}}\left(\ln B_{ij} - \frac{\sum_{t=1}^{n} x_tV_{tj}B_{tj}}{\sum_{l=1}^{n} x_lB_{lj}}\right)\right) \quad (5)$$

where Z_i and Z_j are the nearest molecule or first coordination numbers, and x_i and x_j the molar fractions, and $V_{\mathrm{m}i}$ and $V_{\mathrm{m}j}$ the molar volumes of the matters i and j, respectively; and the pair-potential energy interaction parameters B_{ji} and B_{ij}, respectively, are defined as

$$B_{ji} = \exp\left[-\frac{\varepsilon_{ji} - \varepsilon_{ii}}{kT}\right], \qquad B_{ij} = \exp\left[-\frac{\varepsilon_{ij} - \varepsilon_{jj}}{kT}\right] \quad (6)$$

where ε_{ii}, ε_{jj} and ε_{ji} are the i–i, j–j and i–j pair-potential energies, respectively, and $\varepsilon_{ji} = \varepsilon_{ij}$, and k the Boltzmann constant and T the Kelvin temperature.

3. Modified coordination equation

It is necessary to determine the coordination numbers of liquid metals by applying MIVM to liquid alloys. For the liquid metal, the coordination can be defined as [10]

$$Z_i = 2\int_{r_{0i}}^{r_{\mathrm{m}i}} 4\pi r^2\rho_ig_i(r,T)\,\mathrm{d}r \quad (7)$$

where $\rho_i = N_i/V_i$ and $g_i(r, T)$ are the molecular number density and the radial distribution function, r_{0i} and $r_{\mathrm{m}i}$ the beginning and first peak values of radial distance near its melting point, respectively. Since the coordination decreases exponentially with temperature, $g_i(r, T)$ may be represented as

$$g_i(r,T) = g_i(r)\exp\left(\frac{\alpha\Delta H_{\mathrm{m}i}}{RT}\right) \tag{8}$$

where $\alpha = 1/Z_{\mathrm{c}}$ is a constant and $Z_{\mathrm{c}} = 12$ of close-packed coordination, and $\Delta H_{\mathrm{m}i}$ the melting enthalpy. Suppose that first maximum in the radial distribution function $g_i(r)$ at T (K) approaches a normal distribution, and then when $r = r_{\mathrm{m}i}$, it should be

$$g_i(r_{\mathrm{m}i}) = \frac{r_{\mathrm{m}i}}{(r_{\mathrm{m}i} - r_{0i})\sqrt{2\pi}} \tag{9}$$

Thus, substituting Eqs. (8) and (9) into Eq. (7) and integrating it, one can obtain the equation for the coordination number of a liquid metal

$$Z_i = \frac{2\sqrt{2\pi}}{3}\left(\frac{r_{\mathrm{m}i}^3 - r_{0i}^3}{r_{\mathrm{m}i} - r_{0i}}\right)\rho_i r_{\mathrm{m}i}\exp\left(\frac{\Delta H_{\mathrm{m}i}}{Z_{\mathrm{c}}RT}\right) \tag{10}$$

Suppose that the atoms of the liquid metals are physical particles and the r_{0i} is the distance of closest approach of the atoms, σ_i, and the $r_{\mathrm{m}i}$ the average distance of the atoms at T (K), d_i, approximately, i.e. the former can be obtained from any textbook of crystal chemistry [11], and calculated from

$$d_i = 2 \times 10^{-8}\left(\frac{3V_{\mathrm{m}i}}{0.6022 \times 4\pi}\right)^{1/3} \tag{11}$$

Thus, Eq. (10) becomes

$$Z_i = \frac{2\sqrt{2\pi}}{3}\left(\frac{d_i^3 - \sigma_i^3}{d_i - \sigma_i}\right)\rho_i d_i\exp\left(\frac{\Delta H_{\mathrm{m}i}}{Z_{\mathrm{c}}RT}\right) \tag{12}$$

4. Prediction of the thermodynamic properties of solutes in Pb-based dilute solutions

For a binary mixture i–j, the partial molar excess Gibbs energy of component i is

$$\overline{G}_i^{\mathrm{E}} = \overline{H}_i^{\mathrm{E}} - T\overline{S}_i^{\mathrm{E}} = RT\ln\gamma_i \tag{13}$$

where $\overline{H}_i^{\mathrm{E}}$ and $\overline{S}_i^{\mathrm{E}}$ are the partial molar excess enthalpy and entropy of component i respectively. When $x_i \to 0$, Eq. (13) becomes

$$\ln\gamma_i^{\infty} = \frac{\overline{H}_i^{\mathrm{E}\infty}}{RT} - \frac{\overline{S}_i^{\mathrm{E}\infty}}{R} \tag{14}$$

Suppose that the partial molar infinite dilute excess enthalpy $\overline{H}_i^{\mathrm{E}\infty}$ and entropy $\overline{S}_i^{\mathrm{E}\infty}$ of component i are independent of temperature. Then Eq. (14) may be written as [12]

$$\ln\gamma_i^{\mathrm{E}\infty} = \frac{a}{T} + b \tag{15}$$

where $a = \overline{H}_i^{\mathrm{E}\infty}/R$ and $b = -\overline{S}_i^{\mathrm{E}\infty}/R$. Notice that $\overline{H}_i^{\mathrm{E}\infty}$ is the partial molar infinite dilute mixing enthalpy of component i, $\Delta\overline{H}_i^{\mathrm{M}\infty}$. Based on the Eq. (15) one can estimate the infinite dilute activity coefficient γ_i^{∞} at any temperature from known values $\Delta\overline{H}_i^{\mathrm{M}\infty}$ and $\overline{S}_i^{\mathrm{E}\infty}$.

The activities of solutes in the Pb-based dilute solutions Zn–Bi–Pb, Zn–Cd–Pb and Zn–Sb–Pb at 823 K [13] were chosen to check the validity of Eqs. (5) and (12) since the data is well known to be reliable. In order to determine the required binary parameters B_{ji} and B_{ij}, the some parameters of pure metals and the infinite dilute thermodynamic properties of binary liquid alloys were found for the model as shown in Tables 1 and 2, respectively.

When x_i or x_j approaches zero, the infinite dilution activity coefficients γ_i^{∞} and γ_j^{∞}, respectively, are derived from Eqs. (2) and (3):

$$\ln\gamma_i^{\infty} = 1 - \ln\left(\frac{V_{\mathrm{m}j}B_{ji}}{V_{\mathrm{m}i}}\right) - \frac{V_{\mathrm{m}i}B_{ij}}{V_{\mathrm{m}j}} - \left(\frac{1}{2}\right)(Z_i\ln B_{ji} + Z_jB_{ij}\ln B_{ij}) \tag{16}$$

$$\ln\gamma_j^{\infty} = 1 - \ln\left(\frac{V_{\mathrm{m}i}B_{ij}}{V_{\mathrm{m}j}}\right) - \frac{V_{\mathrm{m}j}B_{ji}}{V_{\mathrm{m}i}} - \left(\frac{1}{2}\right)(Z_j\ln B_{ij} + Z_iB_{ji}\ln B_{ji}) \tag{17}$$

Table 1
Some parameters for the related metals [10,11]

i	σ_i (10^{-8} cm)	$\Delta H_{\mathrm{m}i}$ (kJ/mol)	$V_{\mathrm{m}i}$ (cm^3/mol)
Bi	3.10	10.878	$20.80\,[1 + 1.17 \times 10^{-4}\,(T-544)]$
Cd	2.96	6.109	$14.00\,[1 + 1.50 \times 10^{-4}\,(T-594)]$
Pb	3.48	5.104	$19.42\,[1 + 1.24 \times 10^{-4}\,(T-600)]$
Sb	2.90	19.623	$18.80\,[1 + 1.30 \times 10^{-4}\,(T-903)]$
Zn	2.66	7.364	$9.94\,[1 + 1.50 \times 10^{-4}\,(T-693)]$

Table 2
The infinite dilute thermodynamic properties of the related binary liquid alloys [1]

i–*j*	*T* (K)	$\Delta\overline{H}_i^{\mathrm{M}\infty}$ (kJ mol^{-1})	$\overline{S}_i^{\mathrm{E}\infty}$ (JK^{-1} mol^{-1})	$\Delta\overline{H}_j^{\mathrm{M}\infty}$ (kJ mol^{-1})	$\overline{S}_j^{\mathrm{E}\infty}$ (JK^{-1} mol^{-1})
Bi–Pb	700	−3.489	0.950	−3.460	1.393
Cd–Pb	773	9.326	1.950	15.899	6.849
Sb–Pb	905	0.134	2.230	0.000	2.079
Zn–Pb	923	20.083	4.531	23.012	−4.531
Bi–Zn	873	26.150	0.958	13.577	6.925
Cd–Zn	800	8.828	−0.795	8.786	1.046

The parameter B_{ij} is solved by connecting Eqs. (16) and (17)

$$B_{ij} = \exp(B) \tag{18}$$

$$B = \frac{2}{2+Z_j}\left(1 - \ln\gamma_j^{\infty} - \ln\frac{V_i}{V_j} - \frac{V_j B_{ji}}{V_i} - \frac{1}{2}Z_i B_{ji}\ln B_{ji}\right) \tag{19}$$

Let a function and its derivative be, respectively,

$$f(B_{ji}) = \left(1+\frac{Z_i}{2}\right)\ln B_{ji} + \left(\frac{V_i}{V_j}+\frac{Z_j B}{2}\right)\exp(B) + \ln\left(\frac{V_j}{V_i}\right) + \ln\gamma_i^{\infty} - 1 \tag{20}$$

$$f'(B_{ji}) = \frac{(1+Z_i/2)}{B_{ji}} + \left(\frac{V_i}{V_j}+\frac{Z_j}{2}(1+B)\right)B'\exp(B) \tag{21}$$

$$B' = -\frac{2}{2+Z_j}\left(\frac{V_j}{V_i}+\frac{Z_i\ln B_{ji}}{2}+\frac{Z_i}{2}\right) \tag{22}$$

According to the Newton formulas,

$$B_{ji(n+1)} = B_{ji(n)} - \frac{f[B_{ji(n)}]}{f'[B_{ji(n)}]} \tag{23}$$

and the values of B_{ji} and B_{ij} can be obtained from the γ_i^{∞} and γ_j^{∞} by repeatedly computing until $|B_{ji(n)} - B_{ji(n+1)}| \le 10^{-8}$, as shown in Table 3.

Considering first-order effects only, the Wagner formulae for ternary dilute solutions can be defined as

$$\ln\gamma_i = \ln\gamma_i^{\infty} + x_i\varepsilon_i^i + x_j\varepsilon_i^j \tag{24}$$

where i is the primary solute and j or k the added solute, ε_i^i and ε_i^j are first-order interaction parameters. For Pb-based dilute solutions of Zn–Bi–Pb, Zn–Cd–Pb and Zn–Sb–Pb, the parameters suggested by Pehlke et al. [13], are listed in Table 4.

Allowing the Pb-based dilute solutions Zn–Bi–Pb, Zn–Cd–Pb and Zn–Sb–Pb to be a 1-2-3 system, the activity coefficient of the component 1 of the systems can be written from Eq. (5)

$$\begin{aligned}\ln\gamma_1 = 1 &+ \ln\left(\frac{V_{\mathrm{m}1}}{x_1V_{\mathrm{m}1}+x_2V_{\mathrm{m}2}B_{21}+x_3V_{\mathrm{m}3}B_{31}}\right) - \frac{x_1V_{\mathrm{m}1}}{x_1V_{\mathrm{m}1}+x_2V_{\mathrm{m}2}B_{21}+x_3V_{\mathrm{m}3}B_{31}} \\ &- \frac{x_2V_{\mathrm{m}1}B_{12}}{x_1V_{\mathrm{m}1}B_{12}+x_2V_{\mathrm{m}2}+x_3V_{\mathrm{m}3}B_{32}} - \frac{x_3V_{\mathrm{m}1}B_{13}}{x_1V_{\mathrm{m}1}B_{13}+x_2V_{\mathrm{m}2}B_{23}+x_3V_{\mathrm{m}3}} \\ &- \frac{1}{2}\left(\frac{Z_1(x_2B_{21}+x_3B_{31})(x_2B_{21}\ln B_{21}+x_3B_{31}\ln B_{31})}{(x_1+x_2B_{21}+x_3B_{31})^2} + \frac{Z_2x_2B_{12}[(x_2+x_3B_{32})\ln B_{12}-x_3B_{32}\ln B_{32}]}{(x_1+B_{12}+x_2+x_3B_{32})^2} + \frac{Z_3x_3B_{13}[(x_2B_{23}+x_3)\ln B_{13}-x_2B_{23}\ln B_{23}]}{(x_1B_{13}+x_2B_{23}+x_3)^2}\right)\end{aligned} \tag{25}$$

Substituting the corresponding values for B_{ji} and B_{ij} into Eq. (25), the activities of components of those Pb-based dilute solutions can be predicted, as shown in Tables 5–7. It can be seen from the Tables that the predicted values are in good agreement with the experimental values and the calculated values from the Wagner's formula, respectively, and all the predicting average relative errors $S_1 = (100/n)\sum|(a_{1,\mathrm{exp}} - a_{1,\mathrm{pre}})/a_{1,\mathrm{exp}}|$ are acceptable, where $a_{1,\mathrm{exp}}$ and $a_{1,\mathrm{pre}}$ are the experimental data and the

Table 3
The values of γ_i^∞, γ_j^∞, B_{ji} and B_{ij} of the binary liquid alloys at 823 K

i–j	γ_i^∞	γ_j^∞	B_{ji}	B_{ij}
Zn–Bi	3.163	40.718	1.0879	0.4113
Zn–Cd	3.185	3.998	0.9341	0.8158
Zn–Sb[a]	0.3	0.3	1.0020	1.1854
Zn–Pb	10.916	49.816	0.8521	0.5468
Bi–Pb	0.536	0.510	1.1147	1.0091
Cd–Pb	3.091	4.481	0.9833	0.7655
Sb–Pb	0.780	0.779	1.0176	1.0269

[a] The $\gamma_{\mathrm{Zn}}^\infty$ and $\gamma_{\mathrm{Sb}}^\infty$ obtained from Dealy and Pehlke [14].

Table 4
Some parameters of the Pb-based dilute solutions at 823 K

i–j–k	$\ln \gamma_i^\infty$	ε_i^i	ε_i^j
Zn–Pb	2.437	−3.27	
Zn–Bi–Pb			−0.774
Zn–Cd–Pb			−0.535
Zn–Sb–Pb			−7.901

Table 5
Comparison of the predicted values with the experimental and the calculated values from the Wagner formula of activity of solute Zn in the Zn–Bi–Pb at 823 K

x_{Zn}	x_{Bi}	x_{Pb}	$\ln \gamma_{\mathrm{Zn}}$		
			Eq. (25)[a]	Eq. (24)[b]	Exp. [13]
0.015	0.015	0.970	2.317	2.376	2.468
0.015	0.025	0.960	2.302	2.369	2.451
0.015	0.0375	0.9475	2.284	2.359	2.411
0.015	0.050	0.935	2.266	2.349	2.383
0.025	0.015	0.960	2.284	2.344	2.445
0.025	0.025	0.950	2.270	2.336	2.442
0.025	0.0375	0.9375	2.251	2.326	2.406
0.025	0.050	0.925	2.234	2.317	2.388
0.0375	0.015	0.9465	2.243	2.303	2.418
0.0375	0.025	0.9375	2.229	2.295	2.389
0.0375	0.0375	0.9245	2.211	2.285	2.364
0.0375	0.050	0.9125	2.194	2.276	2.381
0.050	0.015	0.935	2.202	2.262	2.347
0.050	0.025	0.925	2.188	2.254	2.330
0.050	0.0375	0.9125	2.171	2.245	2.310
0.050	0.050	0.900	2.154	2.235	2.310

[a] Eq. (25): $S_1 = \pm 6.39\%$.
[b] Eq. (24): $S_1 = \pm 3.43\%$.

Table 6
Comparison of the predicted values with the experimental and the calculated values from the Wagner formula of activity of solute Zn in the Zn–Cd–Pb at 823 K

x_{Zn}	x_{Cd}	x_{Pb}	$\ln \gamma_{\mathrm{Zn}}$		
			Eq. (25)[a]	Eq. (24)[b]	Exp. [13]
0.015	0.015	0.970	2.318	2.380	2.437
0.015	0.0375	0.9475	2.285	2.368	2.403
0.015	0.050	0.935	2.266	2.361	2.402
0.025	0.015	0.960	2.284	2.344	2.417
0.025	0.025	0.950	2.269	2.342	2.411
0.025	0.0375	0.9375	2.251	2.335	2.388
0.0375	0.015	0.9465	2.242	2.306	2.367
0.0375	0.0375	0.9245	2.209	2.294	2.350
0.0375	0.050	0.9125	2.191	2.288	2.341
0.050	0.015	0.935	2.201	2.266	2.471
0.050	0.025	0.925	2.186	2.260	2.449
0.050	0.050	0.900	2.149	2.247	2.423

[a] Eq. (25): $S_1 = \pm 6.93\%$.
[b] Eq. (24): $S_1 = \pm 3.66\%$.

predicted values of activity of component 1 in a ternary 1-2-3 dilute solutions. This shows that MIVM and the modified coordination equation are quite convenient and reliable for predicting the thermodynamic

Table 7
Comparison of the predicted values with the experimental values and the calculated values from the Wagner formula of activity of solute Zn in the Zn–Sb–Pb at 823 K

x_{Zn}	x_{Sb}	x_{Pb}	$\ln \gamma_{\mathrm{Zn}}$		
			Eq. (25)[a]	Eq. (24)[b]	Exp. [13]
0.015	0.015	0.970	2.287	2.270	2.310
0.015	0.025	0.960	2.252	2.191	2.228
0.015	0.0375	0.9475	2.208	2.092	2.152
0.015	0.050	0.935	2.164	1.993	2.047
0.025	0.015	0.960	2.254	2.237	2.310
0.025	0.025	0.950	2.219	2.158	2.191
0.025	0.0375	0.9375	2.176	2.059	2.138
0.025	0.050	0.925	2.132	1.960	2.061
0.0375	0.015	0.9465	2.213	2.196	2.307
0.0375	0.025	0.9375	2.178	2.117	2.257
0.0375	0.0375	0.9245	2.135	2.018	2.152
0.0375	0.050	0.9125	2.092	1.919	2.070
0.050	0.015	0.935	2.172	2.155	2.293
0.050	0.025	0.925	2.137	2.076	2.223
0.050	0.0375	0.9125	2.095	1.977	2.127
0.050	0.050	0.900	2.052	1.879	2.056

[a] Eq. (25): $S_1 = \pm 2.48\%$.
[b] Eq. (24): $S_1 = \pm 4.69\%$.

properties of the Pb-based ternary dilute solutions that requires only the binary infinite dilute data and provides an important economic advantage since the amount of experimental and computing work required to represent ternary behavior is thereby very much reduced.

5. Conclusions

The coordination numbers in the Molecular Interaction Volume Model can be calculated from common physical quantities of pure metals. A significant advantage of the model lies in its ability to predict the thermodynamic properties of ternary dilute solutions using only the binary infinite dilute activity coefficients, and the predicted values are in good agreement with the experimental data of ternary dilute solutions, which show that the model is reliable, convenient and economic.

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