Statistical thermodynamic approach to molten Fe–Cr–P

Statistical thermodynamic analysis was applied to the available phosphorus solubility data set for molten Fe$_{1-x}$Cr$_x$P$_y$ given as functions of Cr composition y, temperature T and phosphorus activity a(P) under the assumption that the solubility limit x of P in the molten Fe$_{1-x}$Cr was 0.50 irrespective of y. The evaluated values of the energy parameter representing the extent of stability of P atoms in the molten Fe$_{1-x}$Cr$_x$P$_y$ showed an apparently realistic variation pattern with y for the level of y up to 0.465. Further, it was demonstrated by an interpolating estimation using the obtained statistical thermodynamic parameter values at two known levels of y that a(P) vs. x relationships for arbitrary y at specified T could be derived with acceptable accuracy.

Keywords: Molten Fe–Cr–P; Non-stoichiometry; Interstitial compound; Phosphorus activity; Statistical thermodynamics

1. Introduction

Equilibrium a(P)–T–C (phosphorus activity–temperature–composition) relationships for the molten Fe–Cr–P system were determined by Zaitsev et al. [1] using the Knudsen effusion technique over molten Fe$_{1-x}$Cr$_x$P$_y$ for sets of fixed compositions, x and y, by varying temperature T in the range between 1820 K and 1400 K over the range of y between 0.06 and 0.93 and x up to 0.47. The reported discrete set of a(P)–T–C relationships were consisted of totally 84 data points (see Table 1 in Ref. [1] for original data set or Table 1 in Ref. [2] with a converted composition expression in Fe$_{1-x}$Cr$_x$P$_y$ format). Note that xP for the experimental runs 73 ~ 76 in Table 1 of Ref. [2] was mis-typed to be 0.146 in place of the correct 0.143. Such discrete a(P)–T–C data presentation was not very convenient for further thermodynamic or statistical thermodynamic analysis and hence an attempt was made to derive an empirical analytical expression for composition x for given y as functions of T and a(P) in a standardised analytical form [2]

\[ x = A \cdot a(P) \cdot \exp(B \cdot \ln T + C/T) \]  

(1)

This standardised solubility expression was demonstrated to yield values for solubility of H, N and C in the Fe lattice with satisfactory accuracy [3]. In the case of analysis of C solubility in the Fe lattice, the factor B in Eq. (1) was taken to be 0. On the other hand, in the case of analysis of solubilities of H and N in the Fe lattice in the earlier work [3], p(X$_2$)$^{1/2}$ was used to represent a(X).

In the present work, the a(P)–T–C relationships determined experimentally for the molten Fe$_{1-x}$Cr$_x$P$_y$ in the analytical form (1) are analysed using statistical thermodynamics. The results obtained by the present analysis for the molten Fe$_{1-x}$Cr$_x$P$_y$ are compared with the earlier analysis results for molten FeP$_3$ [4] obtained through analysis of solubility data reported by Ban-ya et al. [5, 6] from the equilibration experiment undertaken in P$_2$ gas for compatibility of the estimation results.

2. Analysis procedure and results

2.1. Data sets analysed

As reviewed in the preceding work [2], sets of values for the constants, A, B and C, in the solubility expression (1) were determined for y values, 0.061, 0.114, 0.180, 0.274, 0.376 and 0.465, alone. Other sets of data points containing less than 5 levels of T at a given combination of x and y were not included for the analysis. That is, only the data sets of x and y combinations for which a(P) was specified for at least 5 levels of T were analysed to determine the expression of the normalised format (1) in the preceding preparatory work [2]. The determined values of coefficients, A, B and C, are listed in Table 1. The following statistical thermodynamic analysis is made considering that the numerical a(P)–T–x relationships for given y are determined by Eq. (1) with the parameter values listed in Table 1. At each T for a given y, five sets of a(P) vs. x relations were calculated by choosing an arbitrary value of a(P) to make the

Table 1. Estimated values for the coefficients, A, B and C, in the solubility expression x = A · a(P) · \( \exp(B \cdot \ln T + C/T) \) for molten Fe$_{1-x}$Cr$_x$P$_y$, reproduced from Ref. [2].

<table>
<thead>
<tr>
<th>y</th>
<th>A*10^4</th>
<th>B</th>
<th>C/10^4</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.061</td>
<td>1.030</td>
<td>-1.392&lt;sup&gt;*&lt;/sup&gt;</td>
<td>1.562</td>
</tr>
<tr>
<td>0.114</td>
<td>1.033</td>
<td>-1.411</td>
<td>1.666</td>
</tr>
<tr>
<td>0.180</td>
<td>1.031</td>
<td>-1.424</td>
<td>1.631</td>
</tr>
<tr>
<td>0.274</td>
<td>1.002</td>
<td>-1.406</td>
<td>1.594</td>
</tr>
<tr>
<td>0.375</td>
<td>1.028</td>
<td>-1.342</td>
<td>1.489</td>
</tr>
<tr>
<td>0.465</td>
<td>1.024</td>
<td>-1.223</td>
<td>1.269</td>
</tr>
</tbody>
</table>

<sup>*</sup> The parameter values were taken from Table 2 in Ref. [2] with a correction to the value for B at the composition y = 0.061 which was erroneously determined by a simple careless calculation mistake in converting the composition data given in atom fractions, x(Fe) = 0.155 and x(Cr) = 0.845, to erroneous Fe$_{0.939}$Cr$_{0.061}$P$_0$. Instead of correct Fe$_{0.939}$Cr$_{0.061}$P$_0$.183.
Table 2. Values of \( D(P_2)^{<\circ} \), \( D(P_2)/2 - RT \, C(T) \) and a factor (0.04467 – 117.168) used for the present calculation.

<table>
<thead>
<tr>
<th>( T ) (K)</th>
<th>( D(P_2)^{&lt;\circ} ) (kJ·mol(^{-1}))</th>
<th>( D(P_2)/2 - RT , C(T)^{&lt;\circ} ) (kJ·mol(^{-1}))</th>
<th>0.04467 – 117.168 ( ^{&lt;\circ} ) (kJ·mol(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>1400</td>
<td>247.659</td>
<td>411.920</td>
<td>-54.718</td>
</tr>
<tr>
<td>1500</td>
<td>247.873</td>
<td>425.824</td>
<td>-50.257</td>
</tr>
<tr>
<td>1600</td>
<td>248.090</td>
<td>439.855</td>
<td>-45.796</td>
</tr>
<tr>
<td>1700</td>
<td>248.304</td>
<td>453.998</td>
<td>-41.336</td>
</tr>
<tr>
<td>1800</td>
<td>248.525</td>
<td>468.259</td>
<td>-36.875</td>
</tr>
</tbody>
</table>

\(<\circ> \) \( D(P_2) \) values were taken from JANAF Thermochemical Tables [16] and \( D(P_2)/2 - RT \, C(T) \) was calculated according to Eq. (4). \(<^{\circ}\> \) The factor (0.04467 – 117.168) (kJ·mol\(^{-1}\)) corresponds to \((g - g')\) as expressed in Eq. (10).

2.2. Statistical thermodynamic analysis

In the statistical thermodynamics, the partition function \( PF \) for a condensed phase (either solid or liquid) under consideration is composed taking into account the nearest neighbour atomic interactions. Then, from the partial derivation of \( PF \) with respect to the number \( n_i \) of a constituent element \( i \) in the condensed phase, chemical potential \( \mu(i)^{<\circ} \) of the constituent \( i \) in the condensed phase is derived. Then, \( \mu(i)^{<\circ} \) is put equal to \( \mu(i)^{<\circ} \) of the same element \( i \) in the gas phase.

The expression for \( \mu(X)^{<\circ} \) of an ideal diatomic gas \( X_2 \) is readily available in the classical text book authored by Fowler and Guggenheim [10]. The detailed derivation procedure of \( \mu(X)^{<\circ} \) for the condensed phase MX\(_{s}\) can be referred to elsewhere [11–14]. Anyway, it is essentially reduced to the following set of equations for the purpose of analysing P solution in the present concern [4, 15]

\[
A(T) = RT \ln \left[ \frac{\rho(P_2)}{\rho} \right]^{1/2} \cdot (\theta - x/a) = g + \beta x E(P-P) \\
K = g - \left( \frac{D(P_2)/2 - RT \, C(T)}{Q - RT \, f_0(T)} \right) \\
C(T) = -(1/2) \ln \left[ \left( \frac{4\pi n_{P_2}}{3} \right)^{3/2} \frac{k}{h^3} \right] \\
\times \left[ \frac{T^{7/2}}{\Theta_r} \cdot (1 + \Theta_r/3T) \cdot \left( \frac{\rho^2_0 v_0^2}{2} \right) \right] \\
+ \Theta_r/4T + (1/2) \ln \left[ 1 - \exp(-\Theta_r/T) \right] \\
\ln f_0(T) = - \frac{1}{\rho} \int_0^\infty \left( g(v) \ln \left[ 1 - \exp(-\hbar v/kT) \right] \right) dv + \ln \rho v_0 \\
Q + \beta x E(P-P) = \partial E/\partial n_P
\]

For starting the statistical thermodynamic analysis using Eq. (2), the value for the parameter \( \theta \) must be chosen adequately to yield linear \( A(T) \) vs. \( x \) isotherms. This is to fulfill the a priori assumption of constant \( E(P-P) \) over a range of homogeneity composition \( x \) at a given \( T \) for \( Fe_{1-x}Cr_xP_2 \) of a given composition \( y \). All the past statistical thermodynamic analyses for non-stoichiometric interstitial solution systems were made under this simplifying a priori assumption and the derived conclusions appeared to be realistic being compatible with the other available experimental evidence and so this assumption was considered to be valid although there is no first-principle-based justification to verify the validity of this a priori assumption [2–4, 11–15]. In the earlier analysis for the molten Fe–P system [4], the \( \theta \) value was taken to be 0.50 as pointed out earlier in the text and so the following analysis is made with \( \theta = 0.50 \).

In addition, we need to modify the fundamental statistical thermodynamic formula Eq. (2) expressed as functions of \( \rho(P_2) \), \( T \) and \( x \), to an expression given as functions of \( \alpha(P), T \) and \( x \). By so doing, we can use the present set of data.
presented in form of \( a(P) - T - x \) relationships for given \( y \) rather than in form of \( p(P_2) - T - x \) relationships. For this conversion of the expression of the fundamental formula, the empirical \( p(P_2) - a(P) \) conversion relationship presented by Ban-yau et al. [5] is used.

\[
\log_{10}[p(P_2)^{1/2}/a(P)] = 2.33 - 6120/T
\]

(7)

As this formula was presented in engineering logarithm, it is converted to natural logarithm format to carry out the numerical calculation combined with the fundamental formula Eq. (2).

\[
\ln[p(P_2)^{1/2}/a(P)] = 5.365 - 14092/T
\]

(8)

Then, the fundamental Eq. (2) is converted to the one as functions of \( a(P) \), \( T \) and \( x \) in place of the one as functions of \( p(P_2) \), \( T \) and \( x \)

\[
A'(T) = RT \ln[a(P)] \cdot (\theta - x)/\theta = g' + \beta x E(P-P)
\]

\[
= [g - RT(5.365 - 14092/T)] + \beta x E(P-P)
\]

\[
= (g + 117.168 - 0.0446T) + \beta x E(P-P)
\]

(9)

That is, desired values of \( g \) as a function of \( T \) to evaluate values of \( Q \) and \( R \ln f_P \) using Eq. (3) can be determined from the intercept \( g' \) of \( A' \) vs. \( x \) plot at \( x = 0 \) by the relationship

\[
g = g' + (0.0446T - 117.168) \text{ (kJ \cdot mol}^{-1}\text{)}
\]

(10)

The calculation results for \( A' \) vs. \( x \) relationships at \( T = 1600 \text{ K} \) are plotted in Fig. 1. As seen in Fig. 1, the derived \( A'(T) \) vs. \( x \) isotherm with \( \theta = 0.50 \) at any examined composition \( y \) fell into a linear relationship to fulfill the a priori assumption of constant \( E(P-P) \) in the homogeneity composition range of the molten Fe\(_{1-y}\)Cr\(_y\)P\(_x\). By undertaking similar calculations, the values of the parameters, \( \beta E(P-P) \) and \( g' \), in Eq. (9) for respective \( y \) values were determined as a function of \( T \). These calculation results are presented in Fig. 2 (\( \beta E(P-P) \)) and in Fig. 3 (\( g' \) values).

From the enumerated values of \( g' \), the values of \( g \) were calculated according to Eq. (10) and then the \( K \) vs. \( T \) plots exhibited in Fig. 4 were prepared using Eq. (3). Then, the values of \( Q \) and \( R \ln f_P \) are estimated using values of \([D(P_2)/2 - RT C(T)]\) in Table 2. Calculation results are summarised in Table 3 together with the corresponding values of these parameters for molten FeP\(_x\) reported in the earlier work [4]. To visualise the calculation results, these values are plotted as shown in Fig. 5.

It is seen in Fig. 5 that \( Q \) in the molten Fe\(_{1-y}\)Cr\(_y\)P\(_x\) showed the trend of increasing stability of P with the rising Cr content up to around 0.18 and then, with the further increase in P content, the stability of P in the molten Fe\(_{1-y}\)Cr\(_y\)P\(_x\) tended to become less. The observed trend for variation of \( Q \) against \( y \) in Fig. 5 appears to correspond rationally with the observed rise of P solubility for molten Fe\(_{1-y}\)Cr\(_y\)P\(_x\) with \( y \) increasing from 0 to 0.114 and the decrease in it with the further increase in \( y \) exceeding 0.18 (see Figs. 4 and 5 in Ref. [2]).

According to Zaitsev et al. [9], the congruent melting temperature of the Cr\(_2\)P\(_7\) phase is 1723°C while that of Fe\(_2\)P is 1370°C and the temperature of Cr\(_2\)P melt to be in equilibrium with solid Cr\(_2\)P7 is 1506°C while that of Fe\(_2\)P melt to be in equilibrium with solid Fe\(_2\)P is 1168°C. This evidence appeared to suggest that the P–Cr bond is appreci...
ably tighter than the P–Fe bond and accordingly the observed significant drop in the $Q$ value on the small proportion of alloying with Cr to Fe seen in Fig. 5 appears rational.

Detailed discussion for $R \ln f_P$ is not easy because of its rather complicated dependencies on several atomistic factors but the pattern of variation of it with respect to $y$ appears to demonstrate some systematic change of electronic state around P in the molten Fe$_{1-y}$Cr$_y$P$_x$ with Cr content $y$.

Similar systematic variations of $Q$ and $R \ln f_X$ with respect to the composition $y$ of two metallic constituents (M$_{1-y}$M$_y$)$_x$N$_{1-x}$ were also observed for C solubility in fcc (face centred cubic) Fe$_{1-y}$Co$_y$ and Co$_{1-y}$Ni$_y$ alloy lattices showing smooth transition along the alloy composition across the groups in the Periodic Table of the Elements, Fe through Co to Ni, as exhibited in Fig. 2 in Ref. [17].

This evidence appears to support indirectly the validity of the present statistical thermodynamic analysis as well as the validity of the empirical solubility expression derived in the preceding publication [2].

3. Interpolating estimation of $a(P)$ for given combination of $x$ and $y$ at arbitrary $T$

As reviewed above, the present estimation results looked generally reasonable. Thus, the feasibility of reproducing the experimental data from the estimated set of statistical thermodynamic parameters is examined briefly in the following.

For this, $g'$ and $\beta E(P,P)$ determined for given $y$ on the basis of Eq. (9) are used. That is, we start from

$$RT \ln(a(P) \cdot (0.50 - x)/x) = g' + \beta E(P,P)$$  \hspace{1cm} (11)

By re-writing this equation, we obtain

$$a(P) = \left[ \frac{x}{(0.50 - x)} \right] \cdot \exp \left[ \frac{g' + \beta E(P,P)}{RT} \right]$$  \hspace{1cm} (12)

We undertake the following interpolating estimation using this equation for the data sets, group III containing the test runs Nos. 17–20 and group XV containing the test runs Nos. 80–84 (see Table 4) [1, 2].

As plotted in Fig. 2, $\beta E(P,P)$ values for given $y$ varied with $T$ showing some scatter. To simplify the estimation, we assume that the variation of $\beta E(P,P)$ is roughly represented as a function of $T$ alone

$$\beta E(P,P) = 2.656 - 0.0337T \text{ (kJ mol}^{-1} \text{)}$$  \hspace{1cm} (13)

This equation was determined by simple least-mean-squares fitting of all the data points in Fig. 2.

On the other hand, expressions for $g'$ used for the present estimation are

$$g'(y = 0.180) = -159.228 + 0.0215T \text{ (kJ mol}^{-1} \text{)}$$  \hspace{1cm} (14)

$$g'(y = 0.114) = -155.916 + 0.0165T \text{ (kJ mol}^{-1} \text{)}$$  \hspace{1cm} (15)

The $g'$ values for $y = 0.159$ and $y = 0.130$ are determined by interpolating the constant term and the factor for $T$ independently

$$g'(y = 0.159) = -158.174 + 0.0199T \text{ (kJ mol}^{-1} \text{)}$$  \hspace{1cm} (16)

$$g'(y = 0.130) = -156.719 + 0.0177T \text{ (kJ mol}^{-1} \text{)}$$  \hspace{1cm} (17)

The calculated $a(P)$ values listed in Table 4 were obtained using Eq. (12) by substituting $\beta E(P,P)$ with Eq. (13) and $g'$ with either Eq. (16) or (17).

As seen in Table 4, the calculated values for $a(P)$ for group III data ($y = 0.159$ and $x = 0.050$) were about double that of the experimental values while those for group XV ($y = 0.130$ and $x = 0.325$) were about 4-fold

---

**Table 4. Interpolating estimation of $a(P)$ for molten Fe$_{1-y}$Cr$_y$P$_x$ for given combinations of $y$ and $x$ at arbitrary temperature $T$.**

<table>
<thead>
<tr>
<th>Group #</th>
<th>Run #</th>
<th>Fe$_{1-y}$Cr$_y$P$_x$</th>
<th>$T$ (K)</th>
<th>$a(P)$</th>
<th>experimental</th>
<th>calculated</th>
</tr>
</thead>
<tbody>
<tr>
<td>III</td>
<td>17</td>
<td>Fe$<em>{0.84}$Cr$</em>{0.16}$P$_{0.050}$</td>
<td>1728</td>
<td>0.000008</td>
<td>0.000017</td>
<td></td>
</tr>
<tr>
<td></td>
<td>18</td>
<td></td>
<td>1759</td>
<td>0.000009</td>
<td>0.000020</td>
<td></td>
</tr>
<tr>
<td></td>
<td>19</td>
<td></td>
<td>1787</td>
<td>0.000011</td>
<td>0.000024</td>
<td></td>
</tr>
<tr>
<td></td>
<td>20</td>
<td></td>
<td>1811</td>
<td>0.000012</td>
<td>0.000028</td>
<td></td>
</tr>
<tr>
<td></td>
<td>80</td>
<td>Fe$<em>{0.85}$Cr$</em>{0.15}$P$_{0.325}$</td>
<td>1561</td>
<td>0.000119</td>
<td>0.000026</td>
<td></td>
</tr>
<tr>
<td></td>
<td>81</td>
<td></td>
<td>1603</td>
<td>0.000155</td>
<td>0.000036</td>
<td></td>
</tr>
<tr>
<td></td>
<td>82</td>
<td></td>
<td>1654</td>
<td>0.000204</td>
<td>0.000051</td>
<td></td>
</tr>
<tr>
<td></td>
<td>83</td>
<td></td>
<td>1708</td>
<td>0.000276</td>
<td>0.000073</td>
<td></td>
</tr>
<tr>
<td></td>
<td>84</td>
<td></td>
<td>1812</td>
<td>0.000472</td>
<td>0.000138</td>
<td></td>
</tr>
</tbody>
</table>

---

smaller than the experimental values. These extents of deviations of the calculated $a(P)$ from the corresponding experimental data might be due to the crudeness of the present estimation using coarse approximation for $\beta E(P-P)$ as practiced above using simplifying Eq. (13) while it actually depends on $y$ as well as on $T$. It is easily noticed in Fig. 2 that $\beta E(P-P)$ for different $y$ tended to deviate more widely from the simplifying linear relationship when $T$ increased. Anyway, in spite of the crudeness of the approximation, the order of magnitude of the estimated $a(P)$ was comparable to that of the corresponding experimental data. Thus, the statistical thermodynamic parameter obtained for the molten Fe$_{1-x}$Cr$_x$P$_y$ at different $y$ values might be used to estimate the $a(P)$--$T$--$x$ relationship for arbitrary $y$ level by interpolation to get a rough idea about the correlation between $a(P)$ and $x$ for given $y$ at arbitrary $T$ for molten Fe$_{1-x}$Cr$_x$P$_y$.

In the above brief test, the calculation was made based on $g'$ using Eq. (9) instead of being based on $g$ using Eq. (2). This might be another possible cause leading to the appreciable deviation of the calculated $a(P)$ from the experimental $a(P)$ and the margin of error might be diminished by estimation using $g$ in place of $g'$. 4. Concluding remark

The analytical $a(P)$--$T$--$x$ relationships evaluated for a number of $y$ values for molten Fe$_{1-x}$Cr$_x$P$_y$ in the recent work [2] from the discrete set of $a(P)$--$T$--$x$ data reported by Zaitsev et al. [1] were analysed by statistical thermodynamics.

The results of the statistical thermodynamic analysis appear to be acceptable exhibiting a realistic pattern of variation of the $Q$ parameter with $y$ showing rational correspondence with the observed variation pattern of $P$ solubility in molten Fe$_{1-x}$Cr$_x$P$_y$ although no special tendency of cluster formation by Fe and Cr atoms around the P atom was concluded. Up to $y = 0.18$ in molten Fe$_{1-x}$Cr$_x$P$_y$, the extent of the stabilisation of P atoms in the molten lattice seemed to become higher with increasing $y$ but then, in the range of $y$ higher than 0.18, the extent of the stabilisation of P atoms in the molten lattice seemed to become less with increasing $y$.

It was also demonstrated that the $a(P)$--$x$ relationship for arbitrary composition $y$ at specified temperature $T$ might be estimated with acceptable precision by interpolating simulation using the estimated values of $\beta E(P-P)$ and $g'$ for two known levels of $y$.

The authors are grateful to an anonymous referee assigned by the editor of the journal to peer-review the submitted manuscript for his/her meticulous reading to point out a few numerical calculation errors. His/her constructive comments were invaluable in bringing the originally submitted crude manuscript to this final stage.

**APPENDIX/List of symbols**

\[
\begin{align*}
A(P) & : \text{ chemical activity of P atom} \\
A(T) & : \equiv RT \ln [\{P(P_2)\}^{1/2} \cdot (\theta - \lambda)/\lambda] \text{ (kJ \cdot mol}^{-1}) \text{; calculated from experimentally determined values of} \ P(P_2), T \text{ and} x \text{ for specified value of} \ \theta \ \text{using Eq. (2)} \\
\theta & : \text{number of available interstitial sites for occupation by P atom per metal atom in Fe$_{1-x}$Cr$_x$P$_y$ lattice} \\
\Theta_s & : \text{characteristic temperature for rotation of P$_2$ molecule} \ (= 0.436 \text{ K} <^*1>) \\
\Theta_v & : \text{characteristic temperature for vibration of P$_2$ molecule} \ (= 1123 \text{ K} <^*2>) \\
\mu(X) & : \text{chemical potential of X atom in the condensed phase MX$_x$} \\
\mu(X) & : \text{chemical potential of X atom in the ideal diatomic} \ X_2 \text{ gas molecule} \\
v & : \text{vibrational frequency of P atom in molten Fe$_{1-x}$Cr$_x$P$_y$ lattice} \\
\rho & : \text{nuclear spin weight (taken to be 1)} \\
n_0 & : \text{statistical weight of tightly bound electrons around} \ P \text{ in molten Fe$_{1-x}$Cr$_x$P$_y$ lattice} \\
x_n & : \text{electronic state of P$_2$ molecule in normal state (taken to be 1)} \\
\end{align*}
\]

$<^*1>$ This value of $\Theta_s(P_2) = 0.436 \text{ K}$ was calculated from $B_s = 0.30327 \text{ cm}^{-1}$ listed for ideal diatomic gas P$_2$ in JANAF Thermochemical Tables [16] using a conversion factor 1 cm$^{-1} = 1.4388 \text{ K}$.  

$<^*2>$ This value of $\Theta_v(P_2) = 1123 \text{ K}$ was calculated from $\omega_e = 780.43 \text{ cm}^{-1}$ [16].
N. Shohoji, S. F. Marques: Statistical thermodynamic approach to molten Fe–Cr–P

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(Received June 6, 2007; accepted December 9, 2007)

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DOI 10.3139/146.101630
© Carl Hanser Verlag GmbH & Co. KG
ISSN 1862-5282

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P. Qian, H. Gu, F. Aldinger
Initial stage of bi-modal microstructure in TiO$_2$-doped α-Al$_2$O$_3$ ceramics induced by SiO$_2$ impurity .......... 240

N. Shohoji, S. Figueiredo Marques
Statistical thermodynamic approach to molten Fe–Cr–P .................. 245

Y. Zhou, B. Wang, S. Li, W. Huang, S. Cao
Phase diagram of the iron-rich portion in the iron–aluminium ternary system .................. 251

Isothermal section at 773 K of the Gd–Er–Co ternary system .................. 257

Y. Plevchuk, V. Sklyarchuk, R. Hermann, G. Gerbeth
Thermophysical properties of Nd-, Er-, YNi-alloys .................. 261

P. Berthod
Influence of carbides and of the dendritic orientation on the thermal expansion of Ni-base, Co-base and Fe-base simple cast alloys .......................... 265

Zheng-Rong Zhang, P. Van Houtte, B. Verlinden
Influence of previous ageing treatments on the strength of an Al-4.3 wt.% Mg-1.2 wt.% Cu alloy processed by ECAE .......... 273

A. Chrysanthou, Om Prakash Modi, Li Han, N. Ramakrishnan, J. M. O’Sullivan
Formation and microstructure of (Ti, V)C-reinforced iron-matrix composites using self-propagating high-temperature synthesis .................. 281

K. Frisk, A. Markström
Effect of Cr and V on phase equilibria in Co–WC based hardmetals .................. 287

Zhenmin Du, Cuiping Guo, Mei Tao, Changrong Li
Thermodynamic modeling of the Cu–Se system .................. 294

N. Boutarek, S. Mansour, Sif Eddine Amara, R. Kesri
Phase transition in the Fe–V system .................. 301

S. To, Y. H. Zhu, W. B. Lee
Microstructural changes at the ultra-precision machined surface of Zn–Al based alloy .................. 307

P. D. Zade, A. P. Vanerkar, D. M. Dharmadhikari
Study of structural and electrical properties of arsenic ferries .................. 313

M. H. Asghar, M. Shoabi, S. Naseem, F. Placido
Study of thin film structure based on MgF$_2$, CeO$_2$ and Al$_2$O$_3$ layers for optical applications .................. 322

Notifications
Personal ........................................... 329
News ........................................... 330
Conferences .................................... 338
Imprint ........................................ 338