[Article]

doi: 10.3866/PKU.WHXB201111172

www.whxb.pku.edu.cn

Fe-P 体系热力学再优化

曹战民* 王昆鹏 乔芝郁 杜广巍

(北京科技大学, 钢铁冶金新技术国家重点实验室, 冶金与生态工程学院, 北京 100083)

摘要: 基于最新的实验热力学数据和相图数据, 采用 CALPHAD 技术对 Fe-P 体系进行热力学再优化. 其中, 溶液相(液相、 α -Fe 和 γ -Fe)的 Gibbs 自由能用替换溶液模型描述, 其余化合物(Fe_3P 、 Fe_2P 、 FeP 、 FeP_2 和 FeP_4) 看作严格计量比化合物. 整个优化过程在 Thermo-Calc® 软件包中完成, 优化所得热力学数据和相图信息与实验信息吻合较好, 为 Fe 基合金和含 P 多元合金体系的进一步优化提供了一组自洽可靠的热力学参数.

关键词: Fe-P 体系; CALPHAD 技术; 相图; 热力学优化

中图分类号: O642

Thermodynamic Reoptimization of the Fe-P System

CAO Zhan-Min* WANG Kun-Peng QIAO Zhi-Yu DU Guang-Wei

(State Key Laboratory of Advanced Metallurgy, School of Metallurgical and Ecological Engineering,
University of Science & Technology Beijing, Beijing 100083, P. R. China)

Abstract: The Fe-P binary system was reoptimized by means of the CALPHAD approach. The Gibbs energy descriptions of every phase in the Fe-P binary system were optimized based on the latest experimental thermodynamic and phase diagram data. The solution phase (liquid, α -Fe, and γ -Fe) was described by the substitutional solution approximation and the other phases (Fe_3P , Fe_2P , FeP , FeP_2 , and FeP_4) were treated as the stoichiometric compounds. The optimization was carried out using the Thermo-Calc® software package. The agreement of the optimized phase diagram and thermodynamic data with experimental results is good, and a self-consistent and reliable thermodynamic dataset is obtained to allow further optimization of Fe-based, P-containing multicomponent alloy systems.

Key Words: Fe-P system; CALPHAD approach; Phase diagram; Thermodynamic optimization

1 Introduction

Fe-P is a fundamental binary system of the Fe-based and P-containing multicomponent alloys, which are of great importance for the advanced metallurgy and materials, such as stainless steel, ultra-pure steel refining, and materials design and processing. From thermodynamic point of view, the best optimized parameters of the Fe-P binary system are a quite important basis for thermodynamic optimization of the Fe-based and P-containing multicomponent systems. Also, thermodynamic data of the Fe-P system with strong interactions advance a better understanding of the nature of chemical bonding and inter-

action mechanism. As pointed out by Okamoto¹ in a critical assessment of the Fe-P system, the assessed Fe-P phase diagram was accepted primarily from Kubaschewski² in 1982. Recently, Ohtani *et al.*³ in 2006 and Tokunaga *et al.*⁴ in 2009 evaluated thermodynamic parameters and calculated phase diagram of the Fe-P system in the thermodynamic analysis of the Fe-Ti-P and Fe-Nb-P systems, respectively. But, in both evaluations the valuable thermodynamic properties in the Fe-P system measured by Zaitsev *et al.*⁵ using differential scanning calorimetry and Knudsen effusion method with mass-spectrometric analysis of the gaseous phase were omitted. In order to obtain a set

Received: October 8, 2011; Revised: November 14, 2011; Published on Web: November 17, 2011.

*Corresponding author. Email: zmcao@ustb.edu.cn; Tel: +86-13671040866.

The project was supported by the National Natural Science Foundation of China (50934011).

国家自然科学基金(50934011)资助项目

of self-consistent and reliable thermodynamic description for this binary system, it is necessary to reoptimize the Fe-P system with all available thermodynamic and phase equilibria data using CALPHAD approach^{6,7} and Thermo-Calc[®] software package.⁸

2 Experimental phase diagram data

Due to the practical and theoretical importance many authors investigated the phase equilibria of the Fe-P system. Saklatwalla⁹ firstly published the phase relationship of the Fe-P (0%–24% P, mass fraction) system. Then, Konstantinow¹⁰ and Haughton¹¹ measured the phase diagram of the Fe-P system up to 24% P and 32% P, respectively, and showed the existence of liquid (L) phase and α -Fe, γ -Fe, Fe₃P, Fe₂P, FeP phases. The solubility of P in γ -Fe was measured by several investigators, including Vogel¹² and Roquet *et al.*¹³ using metallography as well as Lorenz¹⁴ and Fisher¹⁵ *et al.* using magnetic measurements, respectively. The assessed maximum solubility of P in γ -Fe is ca 0.56% at 1423 K.^{12,13} The liquidus and solidus of α -Fe were measured by many researchers.^{9,11,16–19} The quantitative values of solid solubility of P in α -Fe were obtained by using metallography,^{11,12,17,20} X-ray analysis,^{21,22} precipitation hardening,²³ lattice parameter measurements,²⁴ electron probe analysis,²⁵ microprobe and micro-hardness tests,²⁶ and X-ray micro-analyzer.²⁷ The experimental results obtained from different investigators established that three invariant reactions exist in the Fe-P system, i.e., $L \rightleftharpoons \alpha\text{-Fe} + \text{Fe}_3\text{P}$, $L + \text{Fe}_2\text{P} \rightleftharpoons \text{Fe}_3\text{P}$, and $L \rightleftharpoons \text{Fe}_2\text{P} + \text{FeP}$. But, as shown in Table 1 there are small differences for the temperature and composition of the invariant points. Franke *et al.*,²⁸ Meisel,²⁹ and Heimbrecht *et al.*³⁰ revealed the existence of FeP₂ by use of density and X-ray diffraction measurements. Holseth *et al.*³¹ measured the maximum homogeneity range of FeP₂ from 65.6% P to 66.9% P and from 66.2% P to 67.1% P, respectively. Jeitschko *et al.*³² synthesized monoclinic FeP₄ from the elements at 927 to 627 °C using iodine as a catalyst and tin as a flux. Up to now, no experimental information about the phase relationship of the Fe-P (0% to 100% P) system was reported.

3 Experimental thermodynamic property data

Weibke *et al.*³³ experimentally measured the formation enthalpies ($\Delta_f H$) of Fe₃P and Fe₂P at 908 K by using an adiabatic calorimeter as well as Lewis *et al.*³⁴ calculated formation enthalpies of Fe₂P, FeP, FeP₂ at 900 K from their temperature dependences of the dissociation pressures measured by Knudsen effusion method. Based on the available thermodynamic and phase equilibria data, Spencer *et al.*³⁵ evaluated the thermodynamic properties of Fe₃P, Fe₂P, FeP, and FeP₂, including heat capacity (C_p), mixing enthalpy ($\Delta_{\text{mix}} H$), formation entropy ($\Delta_f S$), formation enthalpy ($\Delta_f H$), and Gibbs energy of formation ($\Delta_f G$). As mentioned, Zaitsev *et al.*⁵ measured the heat capacities of iron phosphides Fe₃P, Fe₂P, and FeP in the temperature

range of 113–873 K and investigated the thermodynamic properties of iron phosphides (1041–1549 K), bcc solid solution Fe-P (1384–1619 K), and Fe-P liquid alloys (1349–1811 K) by means of Knudsen effusion method with mass-spectrometric analysis of the gaseous phase. Then, based on the experimentally measured results and the second and third thermodynamic laws, $\Delta_f G$ – T relationships of the Fe₃P, Fe₂P, and FeP at 1230–1530 K, $\Delta_f H$, $\Delta_f S$, and $S^\ominus$ (absolute entropy) at 298 K, as well as activities of P in liquid phase and in α -Fe were determined. Little experimental thermodynamic data of FeP₂ and FeP₄ and phase relation information concerning the Fe-P (50%–100%) system existed in literature due to high volatility of phosphorus at elevated temperature. Therefore, the calculated formation enthalpies of FeP₂ and FeP₄ in the Fe-P system at 298 K by first-principles method³ were used as initial values in the present optimization. All thermodynamic data used in the present optimization are summarized in Table 2.

4 Thermodynamic models and optimization

4.1 Reference states

As reference states for the investigated system, the pure solid elements in their stable states at 298.15 K and 10⁵ Pa (stable element reference, SER) were chosen. The Gibbs energy of the element i with Φ phase appears in the following form:

$$\begin{aligned} {}^0G_i^\Phi(T) &= G_i^\Phi(T) - H_i^{\text{SER}}(298.15 \text{ K}) \\ &= a + bT + cT^2 + dT^3 + eT^{-1} + fT \ln T + gT^{-9} \end{aligned} \quad (1)$$

where H_i^{SER} is the enthalpy of the element i in its SER state at 298.15 K and 10⁵ Pa; T is the absolute temperature in K; $G_i^\Phi(T)$ is the Gibbs energy of the element i ; ${}^0G_i^\Phi(T)$ is the molar Gibbs energy of the element i with the structure of Φ referred to the enthalpy of its stable state at 298.15 K and 10⁵ Pa, which is denoted by GHSE*i* when the element i is in its stable state. Different sets of coefficients a to g used in different temperature ranges in Eq.(1) and compiled by the SGTE (Scientific Group Thermodata Europe) database³⁶ were chosen. The used lattice stability parameters for Fe and P are summarized in Table 3.

4.2 Stoichiometric intermetallic compounds

In the Fe-P system intermetallic compounds Fe₃P, FeP, and FeP₄ belong to the stoichiometric phases. Even small solubility of P in Fe₃P and FeP₂ was reported,^{31,37} Fe₃P and FeP₂ were also approximately treated as intermetallic compounds. The Gibbs energy per mole Fe₃P, Fe₂P, and FeP is given as:

$${}^0G_m^\Phi(T) = a + bT + \int_{298.15 \text{ K}}^T C_p dT - T \int_{298.15 \text{ K}}^T \frac{C_p}{T^2} dT \quad (2)$$

where C_p is isobaric molar heat capacity, the coefficients of a and b will be optimized using $\Delta_f H_{298.15 \text{ K}}^\ominus$, $S_{298.15 \text{ K}}^\ominus$ as initial values. The measured values of C_p reported by Zaitsev *et al.*⁵ were also used in the present optimization.

The Gibbs energy per mole FeP₂ and FeP₄ can be expressed as follows:

$${}^0G_m^{\text{Fe}_m\text{P}_n}(T) = m\text{GHSEFe} + n\text{GHSErP} + \Delta_f G^{\text{Fe}_m\text{P}_n} \quad (3)$$

where ${}^0G_m^{\text{Fe}_m\text{P}_n}(T)$ denotes the standard Gibbs energy of forma-

Table 1 Invariant reactions of the Fe-P system

Reaction	Reaction type	P composition in the liquid/%	T/K	Reference
$L \rightleftharpoons \alpha\text{-Fe} + \text{Fe}_3\text{P}$	eutectic	~17	~1253	16 ^a
		16.7	1278	9 ^a
		16.6	1293	10 ^a
		~17	1323	11 ^a
		22.5	1313±10	25 ^a
		~17	1321	18 ^a
		~17	1312	19 ^a
		17	1321	2 ^b
		17.4	1321	1 ^b
		16.7	1320	5 ^b
		16.3	1323	3 ^b
		16.9	1321	35 ^b
		16.5	1324	this work
$L + \text{Fe}_2\text{P} \rightleftharpoons \text{Fe}_3\text{P}$	peritectic	24.4	~1428	10 ^a
		24.2	1439	11 ^a
		24.3	1446	19 ^a
		24.0	1439	2 ^b
		24.0	1439	1 ^b
		24.3	1439	5 ^b
		23.1	1438	3 ^b
		24.5	1439	35 ^b
$L \rightleftharpoons \text{Fe}_2\text{P} + \text{FeP}$	eutectic	23.8	1437	this work
		40	1535	10 ^a
		40	1538	19 ^a
		40	1535	2 ^b
		40	1535	1 ^b
		39.9	1534	5 ^b
		40.4	1533	3 ^b
		40.1	1534	this work
$L \rightleftharpoons \text{Fe}_2\text{P}$	melting point	33.3	1543	9 ^a
		33.3	1623	10 ^a
		33.3	1643	11 ^a
		33.3	1642	this work
$L \rightleftharpoons \text{Fe}_2\text{P} + \text{FeP}$	eutectic	40	1535	11 ^a
		40	1534	this work
$L \rightleftharpoons \text{FeP}$	melting point	50	1724	this work
$L \rightleftharpoons \text{FeP} + \text{FeP}_2$	eutectic	55.9	1660	this work
$L \rightleftharpoons \text{FeP}_2$	melting point	75.0	1799	this work
$L \rightleftharpoons \text{Fe}_2\text{P} + \text{FeP}_4$	eutectic	73.2	1750	this work
$L \rightleftharpoons \text{FeP}_4$	melting point	80	1799	this work
$L \rightleftharpoons \text{red_P} + \text{FeP}_4$	eutectic	~100	852	this work

^ameasured; ^bassessed

tion per mole formula of Fe_mP_n . Due to the lack of experimental data of heat capacities, by applying to the Neumann-Kopp rule, $\Delta_f G^{\text{Fe}_m\text{P}_n}$ can be given as follows:

$$\Delta_f G^{\text{Fe}_m\text{P}_n} = a + bT \quad (4)$$

where the parameters a and b were to be evaluated in the present work.

4.3 Solution phases

There are three solution phases in the Fe-P system, i.e., liquid phase, bcc (α -Fe), and fcc (γ -Fe). The Gibbs energy of the

solution phase in the Fe-P system is described as follows:

$${}^0G_m^\phi = x_{\text{Fe}} {}^0G_{\text{Fe}}^\phi(T) + x_{\text{P}} {}^0G_{\text{P}}^\phi(T) + RT(x_{\text{Fe}} \ln x_{\text{Fe}} + x_{\text{P}} \ln x_{\text{P}}) + {}^E G_m^\phi \quad (5)$$

where ${}^E G_m^\phi$ is excess molar Gibbs energy, which can be expressed by Redlich-Kister polynomial³⁸ as,

$${}^E G_m = x_{\text{Fe}} x_{\text{P}} \left[L_0 + (x_{\text{Fe}} - x_{\text{P}}) L_1 + (x_{\text{Fe}} - x_{\text{P}})^2 L_2 \right] \quad (6)$$

where L_i ($i=0, 1, 2, \dots$) are the i -order interaction parameters of liquid phase in the Fe-P system and are expressed as temperature dependent terms as follows:

Table 2 Thermodynamic data in the Fe-P system (reference states: α -Fe and red_P)

Thermodynamic function	Phase	Method	Value	Reference
$C_p(\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1})$	Fe_3P	DSC	$27.725+2.925\times 10^{-3}T-2.6975\times 10^3T^{-2}$ (298–633 K)	5
			$(21.40\pm 0.29)+(1.125\pm 0.173)\times 10^{-2}T$ (713–873 K)	5
$C_p(\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1})$	Fe_2P	DSC	$(22.22\pm 0.24)+(9.6\pm 0.4)\times 10^{-3}T$ (298–873 K)	5
$C_p(\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1})$	FeP	DSC	$(21.13\pm 0.175)+(1.05\pm 0.03)\times 10^{-2}T$ (298–873 K)	5
$S_{298\text{ K}}^\ominus(\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1})$	Fe_3P	the third law calculation	29.3±2.7	5
		C_p measurements	27.4±2.0	5
		the third law calculation	25.4±3.1	35
$S_{298\text{ K}}^\ominus(\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1})$	Fe_2P	the third law calculation	28.8±2.2	5
		C_p measurements	30.2±1.7	5
		the third law calculation	24.1±2.8	35
$S_{298\text{ K}}^\ominus(\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1})$	FeP	the third law calculation	25.4±3.3	5
		C_p measurements	28.5±2.5	5
$\Delta_f H_{298\text{ K}}^\ominus(\text{kJ}\cdot\text{mol}^{-1})$	Fe_3P	the second law analysis	-35.1±2.4	5
		the second law analysis	-36.7±2.1	35
		first-principles calculations	-48.4	3
$\Delta_f H_{1200\text{ K}}^\ominus(\text{kJ}\cdot\text{mol}^{-1})$	Fe_3P	the second law analysis	-39.0	5
$\Delta_f H_{908\text{ K}}^\ominus(\text{kJ}\cdot\text{mol}^{-1})$	Fe_3P	calorimetric measurement	-36.8	33
$\Delta_f H_{298\text{ K}}^\ominus(\text{kJ}\cdot\text{mol}^{-1})$	Fe_2P	the second law analysis	-46.2±2.2	5
		the second law analysis	-47.6±2.8	35
		first-principles calculations	-54.6	3
$\Delta_f H_{900\text{ K}}^\ominus(\text{kJ}\cdot\text{mol}^{-1})$	Fe_2P	Knudsen effusion	-49.1	34
$\Delta_f H_{908\text{ K}}^\ominus(\text{kJ}\cdot\text{mol}^{-1})$	Fe_2P	calorimetric measurement	-48.1	33
$\Delta_f H_{1200\text{ K}}^\ominus(\text{kJ}\cdot\text{mol}^{-1})$	Fe_2P	the second law analysis	-50.0	5
$\Delta_f H_{298\text{ K}}^\ominus(\text{kJ}\cdot\text{mol}^{-1})$	FeP	the second law analysis	-52.5±3.5	5
		the second law analysis	-60.4±6.3	35
		first-principles calculations	-82.5	3
$\Delta_f H_{900\text{ K}}^\ominus(\text{kJ}\cdot\text{mol}^{-1})$	FeP	Knudsen effusion	-59.9	34
$\Delta_f H_{1200\text{ K}}^\ominus(\text{kJ}\cdot\text{mol}^{-1})$	FeP	the second law analysis	-55.1	5
$\Delta_f H_{298\text{ K}}^\ominus(\text{kJ}\cdot\text{mol}^{-1})$	FeP_2	the second law analysis	-62.2±5.7	35
		first-principles calculations	-95	3
$\Delta_f H_{900\text{ K}}^\ominus(\text{kJ}\cdot\text{mol}^{-1})$	FeP_2	Knudsen effusion	-60.8±2.8	34
$\Delta_f H_{298\text{ K}}^\ominus(\text{kJ}\cdot\text{mol}^{-1})$	FeP_4	first-principles calculations	-87.1	3

Table 3 Lattice stability parameters used in the present optimization

Element	Phase	Lattice stability parameter	T/K	Reference
Fe	L	${}^0G_{\text{Fe}}^\text{L}-{}^0G_{\text{Fe}}^\text{L}=12040.17-6.55843T-3.6751551\times 10^{-21}T^7$	298.15–1811	36
		$=-10839.7+291.302T-46T\ln T$	1811–6000	36
	α	${}^0G_{\text{Fe}}^\alpha-{}^0H_{\text{Fe}}^\alpha=1225.7+124.134T-23.51437\ln T-0.00439752T^2-5.8927\times 10^{-8}T^3+77359T^4$	298.1–1811	36
		$=-25383.581+299.31255T-46T\ln T+2.29603\times 10^{31}T^9$	1811–6000	36
	γ	$T_{\text{Fe}}^\alpha=1043, \beta_{\text{Fe}}=2.22$	298.15–6000	36
		${}^0G_{\text{Fe}}^\gamma-{}^0H_{\text{Fe}}^\gamma=-1462.4+8.282T-1.157\ln T+6.4\times 10^{-4}T^2$	298.15–1811	36
		$=-27098.266+300.25256T-46T\ln T+2.78854\times 10^{31}T^{-9}$	1811–6000	36
		$T_{\text{Fe}}^\gamma=67, \beta_{\text{Fe}}=0.7$	298.15–6000	36
	P	${}^0G_{\text{Fe}}^\text{L}-{}^0H_{\text{Fe}}^\text{white}=-26316.111+434.943931T-70.74405847\ln T-0.002898936T^2+3.9049341\times 10^{-5}T^3+1141.47T^{-1}$	275–342.3	36
		$=-7232.449+133.304873T-26.326T\ln T$	342.3–6000	36
P	α	${}^0G_{\text{P}}^\alpha-{}^0H_{\text{P}}^\alpha=44769-13.26T$	298.15–6000	36
		${}^0G_{\text{P}}^\gamma-{}^0H_{\text{P}}^\gamma=37656-13.26T$	298.15–6000	36
	red	${}^0G_{\text{P}}^\text{red}-{}^0G_{\text{P}}^\text{white}=-25976.559+148.685002T-25.557\ln T+0.0034121T^2-2.418867\times 10^{-6}T^3+160095T^{-1}$	275–500	36
		$=-21723.721+77.684737T-14.3687\ln T-0.00957685T^2+3.93917\times 10^{-7}T^3-141375T^{-1}$	500–852.35	36
		$=-119408.413+1026.04262T-149.4495567\ln T+0.067272364T^2-6.651929\times 10^{-6}T^3+1249543T^{-1}$	852.35–1500	36
		$=-24524.119+153.852181T-26.326T\ln T$	1500–3000	36
	white	${}^0G_{\text{P}}^\text{white}-{}^0H_{\text{P}}^\text{white}=-43821.799+1026.70689T-178.4267\ln T+0.290708T^2-1.04022667\times 10^{-4}T^3+1632695T^{-1}$	250–317.3	36
		$=-9587.448+152.354487T-28.73353017\ln T+0.0017156697T^2-2.2829\times 10^{-7}T^3+172966T^{-1}$	317.3–900	36
		$=-8093.075+135.889831T-26.326T\ln T$	900–3000	36

G and H are in $\text{J}\cdot\text{mol}^{-1}$, T_c and T_N are Curie temperature and Neel temperature in K, respectively, and β is magnetic moment in $\text{J}\cdot\text{T}^{-1}$.

Fig.4 Calculated heat capacity of Fe_3P (a), Fe_2P (b), and FeP (c) with the literature data

Fig.5 Calculated absolute entropy in the Fe-P system with the literature data

and the previous results assessed by Okamoto¹ and Ohtani *et al.*³ As the part of Fe-P (50%–100% P), there is no experimental information compared with calculated phase diagram. But, if compared the present calculated phase diagram with the previous assessed one,³ the former is a little more reasonable than the latter.

Fig.2 compares the calculated values of formation enthalpies of the Fe-P system at 298 and 900 K in this study with the literature data. Obviously, the present calculated values are in good agreement with measured⁵ and evaluated³⁵ data at 298 K as well as with measured data at 900 K.^{33,34} However, the values evaluated by Ohtani *et al.*³ and Tokunaga *et al.*⁴ and predicted using first-principles calculations³ are more negative than the experimental measured data.⁵

Fig.3 presents the calculated $\Delta_{\text{mix}}H$ of liquid Fe-P system at 1809 K compared with the experimental data.^{3,4,35} It is clear that the present calculated values agree well with evaluated data by Spencer *et al.*³⁵

It can be seen from Fig.4 and Fig.5 that agreement between present calculated heat capacities and absolute entropies of Fe_3P , Fe_2P , and FeP with measured data⁵ is better than the one between previous evaluated data^{3,4} with measured data.⁵

6 Conclusions

Based on all available experimentally measured thermody-

namic properties and phase diagram data, the Fe-P system, which is a significant binary one of the Fe-based and P-containing multicomponent alloys, was reoptimized by CALPHAD approach and Thermo-Calc[®] software package. The agreement between the optimized Fe-P (0%–50% P) phase diagram and experimentally measured data is good enough. The calculated Fe-P (50%–100% P) phase diagram is a little more reasonable than previously assessed one. The comparison of calculated formation entropies of the Fe-P system at 298 and 900 K, calculated mixing entropies of the Fe-P system at 1809 K as well as calculated heat capacities of Fe_3P , Fe_2P , and FeP in this study with the measured data available from literature remains fairly good. An obtained thermodynamic description with self-consistency describing all the phases in the Fe-P system is better than that of the previous assessment.

References

- (1) Okamoto, H. *Bulletin of Alloy Phase Diagrams* **1990**, *11*, 404.
- (2) Kubaschewski, O. *Iron-Binary Phase Diagrams*; Springer-Verlag: Berlin, 1982; pp 84–86.
- (3) Ohtani, H.; Hanaya, N.; Hasebe, M.; Teraoka, S.; Abe, M. *CALPHAD* **2006**, *30*, 147.
- (4) Tokunaga, T.; Hanaya, N.; Ohtani, H.; Hasebe, M. *ISIJ International* **2009**, *49*, 947.
- (5) Zaitsev, A. I.; Dobrokhotova, Z. V.; Litvina, A. D.; Mogutnov, B. M. *J. Chem. Soc. Faraday Trans.* **1995**, *91*, 703.
- (6) Kaufman, L.; Bernstein, H. *Computer Calculation of Phase Diagrams*; Academic Press: New York, 1970.
- (7) Saunders, N.; Modwnik, A. P. *CALPHAD—a Comprehensive Guide*; Pergamon, Lausanne: Switzerland, 1998.
- (8) Sundman, B.; Jansson, B.; Anderson, J. O. *CALPHAD* **1985**, *9*, 153.
- (9) Saklatwalla, B. J. *Iron Steel Inst.* **1908**, *77*, 92.
- (10) Konstantinow, N. Z. *Anorg. Chem.* **1910**, *66*, 209.
- (11) Haughton, J. L. *J. Iron Steel Inst.* **1927**, *115*, 417.
- (12) Vogel, R. *Arch. Eisenhüttenwes.* **1929–1930**, *3*, 369.
- (13) Roquet, P.; Jegaden, G. *Rev. Metall.* **1951**, *48*, 712.
- (14) Lorenz, K.; Frabritius, H. *Arch. Eisenhüttenwes.* **1962**, *33*, 269.

- (15) Fisher, W. A.; Lorenz, K.; Fabritius, H.; Hoffmann, A.; Kalwa, G. *Arch. Eisenhüttenwes.* **1966**, 37, 79.
- (16) Gercke, E. *Metallurgie* **1908**, 5, 604.
- (17) Hanemann, H.; Voss, H. *Zentr. Hutten. Walzwerke* **1927**, 31, 245.
- (18) Wachtel, E.; Urbain, G.; Ubelacker, E. *Compt. Rend.* **1963**, 257, 2470.
- (19) Schürmann, E.; Kaiser, H. P.; Hensgen, U. *Arch. Eisenhüttenwes.* **1981**, 52, 51.
- (20) Kaneko, H.; Nishizawa, T.; Tamaki, K.; Tanifuji, A. *Nippon Kinzoku Gakkai-Shi* **1965**, 29, 166.
- (21) Kreutzer, C. Z. *Phys.* **1928**, 48, 556.
- (22) Oberhoffer, P.; Kreutzer, C. *Arch. Eisenhüttenwes.* **1929**, 2, 449.
- (23) Yensen, T. D. *Trans. Am. Inst. Elec. Eng.* **1924**, 43, 145.
- (24) Svechnikov, V. N.; Pan, V. M. *Phys. Met. Metallogr.* **1958**, 6, 80.
- (25) Doan, A. S., Jr.; Goldstein, J. I. *Metall. Trans.* **1970**, 1, 1759.
- (26) Hofman, H. P.; Lohberg, K.; Reif, W. *Arch. Eisenhüttenwes.* **1970**, 41, 975.
- (27) Ko, M.; Nishizawa, T. *Jpn. Inst. Met.* **1979**, 43, 118.
- (28) Franke, W.; Meisel, K.; Juza, R. *Z. Anorg. Chem.* **1934**, 218, 346.
- (29) Meisel, K. *Z. Anorg. Chem.* **1934**, 218, 360.
- (30) Heimbrecht, M.; Biltz, W. *Z. Anorg. Chem.* **1939**, 242, 233.
- (31) Holseth, H.; Kjekshus, A. *Acta Chemica Scandinavica* **1968**, 22, 3273.
- (32) Jeitschko, W.; Braun, D. *J. Acta Crystallogr. B* **1978**, 34, 3196.
- (33) Weibke, F.; Schrag, G. *Elektrochemische Kinetik* **1941**, 47, 222.
- (34) Lewis, G.; Myers, C. E. *J. Phys. Chem.* **1963**, 67, 1289.
- (35) Spencer, P.; Kubaschewski, O. *Arch. Eisenhüttenwes.* **1978**, 49, 225.
- (36) Dinsdale, A. T. *CALPHAD* **1991**, 15, 317.
- (37) Carsson, B.; Golin, M.; Rundqvist, S. *J. Solid State Chem.* **1973**, 8, 57.
- (38) Redlich, O.; Kister, A. T. *Ind. Eng. Chem.* **1948**, 40, 345.

中国化学会第28届学术年会通知

中国化学会第28届学术年会将于2012年4月13–16日在四川省成都市举行。本届年会由中国化学会主办,四川大学承办,会期4天,4月12日报到。2012年正值中国化学会成立八十周年,届时将举办相关庆祝活动。

本届年会设立学术分会19个、专题论坛4个。学术交流形式包括大会特邀报告(PL)、分会邀请报告(I)、口头报告(O)和墙报(P)。年会面向全国广大化学工作者征集学术论文(摘要),并印制论文摘要集,欢迎踊跃投稿,积极参会。

年会期间将举办新技术、新产品与新仪器成果展览以及人才交流活动,欢迎相关企业、高校、科研院所积极参与。

会议详细内容请见会议网站: <http://www.ccs.ac.cn/confab/huiyi.html>