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New Thermodynamic Assessment of the Fe-Y System

I. Saenko[1,2] · O. Fabrichnaya[1] · A. Udovsky[2,3]

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Abstract Critical review of the Fe-Y binary system has been performed and available experimental and calculated data have been collected. Thermodynamic parameters were optimized using the CALPHAD method. New experimental results of Gibbs energy and Ab-initio calculations of enthalpy of formation of intermetallic compounds have been taken into account. A self-consistent thermodynamic description of the Fe-Y system has been obtained. Problems of thermodynamic modelling in this system have been discussed. The results calculated using thermodynamic descriptions derived in the present work are compared with ones previously published using general "χ^2"-criterion. This criterion allows taking into account the number independent optimized parameters used in the optimization. The calculated agreement criterion has shown that thermodynamic description of the present work describes experimental data better than earlier published ones.

Keywords CALPHAD · Fe-Y binary system · phase diagram · thermodynamic modeling

✉ I. Saenko
ivan.saenko@iww.tu-freiberg.de

[1] Institute of Materials Science, Technical University Bergakademie Freiberg, Gustav-Zeuner-Str. 5, 09599 Freiberg, Germany

[2] A.A. Baikov Institute of Metallurgy and Materials Science, Russian Academy of Sciences, Leninskiy Prospect 49, Moscow, Russia 119991

[3] National Research Nuclear University MEPhI, Kashirskoye sh., 31, Moscow, Russia 115409

1 Introduction

Rare-earth intermetallic compounds based on the Fe-Y system are of particular interest due to their potential industrial applications, such as permanent magnets, as well as hydrogen storage materials.[1,2] Knowledge of phase relations and thermodynamic properties of the Fe-Y system is important for understanding of technological aspects of design and usage of materials and alloys based on the Fe-Y binary system. Moreover, thermodynamic assessment of the Fe-Y binary system can play an important role as subsystem for investigations and modelling of high-order systems, for example, for the modelling interaction strengthened ferrite steels by the oxide dispersion.[3] Du et al.[4] were the first who performed thermodynamic assessment of the Fe-Y system using CalPhaD method. There were several inconsistencies between experimental and calculated data on phase relations as well as thermodynamic properties. After that, thermodynamic modeling of Fe-Y system was carried out by Gong et al. in the frame of the thermodynamic investigation of the Fe-Ti-Y ternary system.[5] The thermodynamic parameters for the Fe-Y system were optimized based on the phase diagram evaluation of Zhang et al.[6] However, no parameters were published. Then calculated phase diagrams of Fe-Y system were independently presented by Lu et al.[7] and Kardellass et al.[8] without publishing of optimized thermodynamic parameters. Afterwards, full thermodynamic assessment and thermodynamic modeling of the iron–yttrium system were published by Kardellass et al.[9] However, Ab-initio calculation of enthalpy[10] and experimental results[11] of Gibbs energy of formation for intermetallic compounds were not taken into account. The last thermodynamic assessment was performed by Konar et al. in the work.[12] This work was an extended doctor thesis of Konar[13] and

taken into account all available experimental data except of Ab-initio calculation of Mihalkovic and Widom.[10] It should be mentioned that in the works of Konar et al.[12,13] the modified quasichemical model was applied for the liquid phase while intermetallic phases were described as stoichiometric compounds. However the modified quasichemical model is not compatible with the substitutional model. Therefore, the aim of this work is to assess the thermodynamic parameters for the Fe-Y system taking into account new experimental results[11] and Ab-initio calculations[10] resulting in a thermodynamic description, which could be applied for the further thermodynamic modeling of high-order systems.

2 Experimental Data in the Fe-Y System

Firstly, phase relationships in the Fe-Y system were investigated in the work of Domagala et al.[14] and in the work of Farkas and Bauer.[15] Domagala et al.[14] have studied the entire composition range of the system using thermal-, x-ray and microscopical analyses using very pure starting materials. Iron was stated to be 99.9% pure, and yttrium 99.0% pure. Major impurities of yttrium were 0.5% of Zr, 0.2% of Ti and 0.12% of O. Specimens were produced using arc-melting and subsequently homogenized. Farkas and Bauer[15] investigated only Fe-rich region (about 70-100 wt.% Fe). Results obtained by these two research groups are in conflict with each other in the Fe-rich region. Farkas and Bauer[15] used less pure component metals in comparison with the work,[14] and specimens were not homogenized. Therefore, basic diagram proposed by Domagala et al.[14] was accepted as more accurate one by Gscheidner[16] and later by Kubuschewski[17] in the first critical reviews of the Fe-Y system. However, Gscheidner assumed that accuracy of the experimental technique employed by Domagala et al.[14] was not enough to provide very reliable results. Further, Kubuschewski[17] corrected phase stoichiometry in order to bring the diagram into accordance with more recent results of crystallographic investigation. The version of the phase diagram presented by Kubuschewski[17] with few corrections based on original data of Domagala et al.[14] is shown in the Fig. 1. The last evaluation of the experimental data was performed by Zhang et al.[6] This work was mostly focused on the recent crystal structure data, magnetic and thermodynamic properties, but not on the phase relations. Data on the solubility of the solid phases in the Fe-Y system, existence of metastable phase, crystal structures and lattice parameters of the intermetallic compounds, their magnetic properties, experimental results of mixing enthalpy of liquid phase and the Gibbs energy of formation of compounds were summarized and reviewed.

According to actual information state, there are four intermetallic compounds in the Fe-Y system, namely $Fe_{17}Y_2$, $Fe_{23}Y_6$, Fe_3Y, and Fe_2Y. The reported compound "Fe_5Y" with $CaCu_5$ structure[16] was not confirmed by the later experimental investigation of Taylor and Poldy.[19] In the work of Tenhover,[20] amorphous alloys were prepared by splat-cooling of Fe-Y liquid with 32 at.% of yttrium and metastable phases were observed. It was shown that the crystallization of this glassy alloy occurs in two distinct steps associated with the formation of hcp(Y) and the Laves phase compound Fe_2Y. A bcc phase was observed in the Y rich Fe-Y alloys rapidly quenched by a melt spinning technique, as well as in the alloys close to eutectic composition of the Fe-Y equilibrium phase diagram (34.6 at.% of Fe).[20]

Some of the stable phases, namely $Fe_{17}Y_2$ and $Fe_{23}Y_6$, earlier were considered to be "Fe_9Y" and "Fe_4Y," respectively according to Domagala et al.[14] In the further crystallographic study of Kripyakevich et al.,[21] it was shown that Fe_9Y phase had an ideal stoichiometry of hexagonal $Ni_{17}Th_2$-type structure. Then, a structure investigation by Buschow[22] revealed that $Fe_{17}Y_2$ had two modifications: the rhombohedral Th_2Zn_{17} type and the hexagonal Th_2Ni_{17} type. It was observed, that the samples annealed at 1273 K for 15 days contained both types of $Fe_{17}Y_2$, while the splat-cooled sample contained only the hexagonal type.[22] Therefore, the hexagonal phase should be the high-temperature modification of the compound $Fe_{17}Y_2$. According to the investigation of Domagala et al.,[14] this compound melts congruently at 1673 ± 25 K. It should be mentioned, that the temperature of this transformation was not determined experimentally. Independent investigations of Kripyakevich et al.[21] and Kharchenko et al.[23] have defined that Fe_4Y has an ideal stoichiometry of $Fe_{23}Y_6$ which is isomorphous to $Mn_{23}Th_6$. This intermetallic compound has fcc crystal structure with 116 atoms per unit cell. Their arrangement of atoms was described in detail by Smith et al.[24] According to the work of Domagala et al.,[14] $Fe_{23}Y_6$ melts congruently. Initially, possible existence of Fe_3Y phase was reported by Domagala et al.[14] They mentioned that the alloy of this composition always contained two or three phases and that no alloy could be prepared being free of segregation. Therefore, it was difficult to confirm the existence of this compound as a stable phase. Later it was established by van Vucht[25] and Buschow[26] that Fe_3Y was a stable phase isomorphous to $PuNi_3$. Domagala et al.[14] reported that Fe_3Y melts congruently at about 1673 K. Kubuschewski[17] considered this melting temperature as too high. Fe_2Y is the Laves phase having cubic with $MgCu_2$-type structure. This compound formed peritectically and showed a narrow homogeneity range.[14,27] The crystal structure of Fe_2Y was

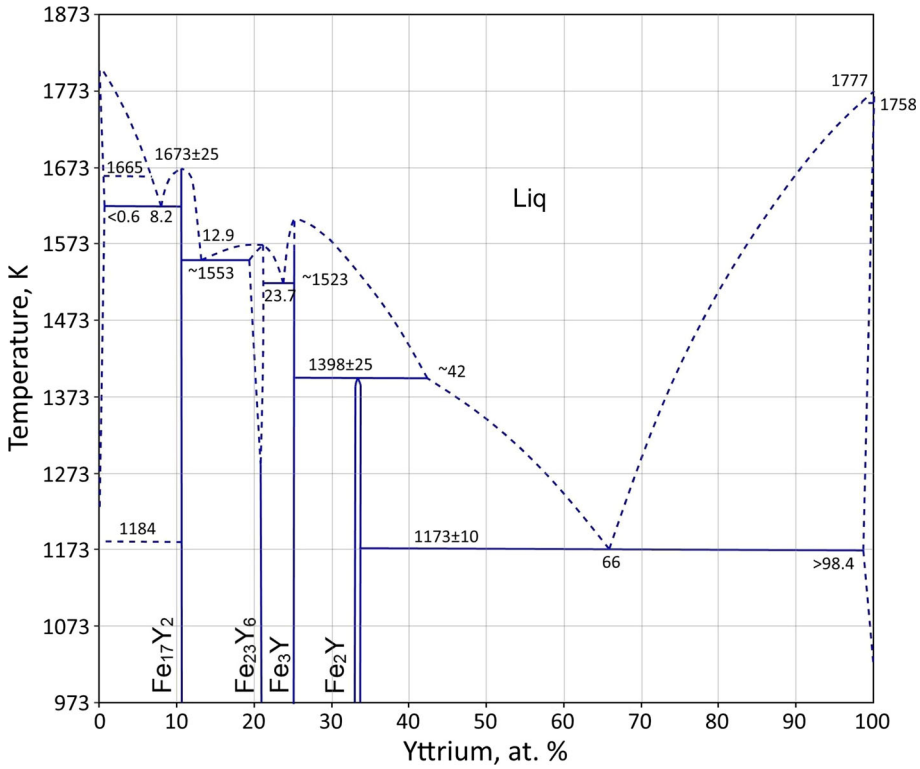

Fig. 1 Phase diagram of the Fe-Y system[14,17,18]

described in detail in the work of Dwight.[28] The crystal structures of all solid phases are listed in the Table 1.

Hellawell[29] reported that 1 at.% of yttrium lowers the γ/δ Fe transformation temperature by 3 K. The effect of yttrium on the α/γ Fe transformation is not known.[17] However, solubility of yttrium in αFe was measured by Li and Xhing[31] using EPMA (electron probe microanalysis) in the temperature interval of 873-1153 K. The experimental results were presented by the relationship: $\ln(X_{\text{at.\%of}Y}) = -2363.7/T(\text{K}) - (5.892 \pm 0.060)$. The terminal solid solubility of Y in γFe was not measured and Gscheidner[16] assumed them to be less than 0.6 at.%.

The first thermodynamic data was experimentally obtained in the work of Ryss et al.[32] They measured the mixing enthalpy of liquid Fe-Y alloys at temperature of 1600 K. The data was obtained in the entire composition range with a step of 5 at.%. The results showed a negative deviation from ideal behavior with a minimum of integral enthalpy of -8.44 kJ mol^{-1} at 47 at.% of Y. Later, partial enthalpy of mixing in the Fe rich liquid was measured by Sudavtsova et al.[33] indicating less negative deviations from ideal behavior than obtained by Ryss et al.[32]

Nagai et al.[34] measured yttrium and iron activities using the multi-Knudsen cell mass spectrometry in the temperature range of 1473-1573 K with pure elements as reference substances. The Fe-Y alloys were prepared using reagent grade yttrium (99.99%) and electrolytic iron (99.99%).

Table 1 Data on crystal structures of solid phases of the Fe-Y system

Phase	Crystal system	Space group	Pearson symbol	Prototype	Reference
αFe	Cubic	$Im\bar{3}m$	cI2	W	18
γFe	Cubic	$Fm\bar{3}m$	cF4	Cu	18
δFe	Cubic	$Im\bar{3}m$	cI2	W	18
$\alpha Fe_{17}Y_2$	Hexagonal	$P6_3/mmc$	hP*	$Ni_{17}Th_2$	21, 22
$\beta Fe_{17}Y_2$	Trigonal	$R\bar{3}m$	hR*	Th_2Zn_{17}	22
$Fe_{23}Y_6$	Cubic	$Fm\bar{3}m$	cF116	$Mn_{23}Th_6$	21, 23, 24
Fe_3Y	Trigonal	$R\bar{3}m$	hR*	$PuNi_3$	25, 26
Fe_2Y	Cubic	$Fd\bar{3}m$	cF24	Cu_2Mg	29, 30
αY	Hexagonal	$P6_3/mmc$	hP2	Mg	16, 18
βY	Cubic	$Im\bar{3}m$	cI2	W	16, 18

Firstly, the Gibbs energies of phase formation for $Fe_{17}Y_2$, $Fe_{23}Y_6$, Fe_3Y, and Fe_2Y were determined by Subramanian and Smith[35] using EMF (electro motive force) method in the temperature range of 893-1271 K. Enthalpies and entropies of formation of phases were obtained by second law evaluation of EMF data. The further experimental evaluation of the enthalpy and entropy of formation of $Fe_{17}Y_2$ was performed by Gozzi et al.[11] based on EMF measurements. Comparison of the obtained results with the previous results showed good agreement of Gibbs energies of formation, as well as, enthalpies and entropies. However, the measurement was carried out also only in the narrow temperature range from 825 up to 980 K and enthalpies and entropies of formation of phases were evaluated by the second law as well. Watson and Bennett[36] used a simple Friedel-type d-band model in order to predict enthalpies of formation of Fe-Y phases. The predicted value for the ficticious compound FeY was of the order of -42 kJ mol^{-1} (values are given per mole of atoms)[36] and later was re-evaluated to be equal to -13 kJ mol^{-1}.[37] In contrast, the Miedema theory[38] predicted the enthalpies of formation of Fe-Y phases to be of the order lower and was calculated as -2 kJ mol^{-1}.[39] However, these calculations differ from experimental values of Subramanian and Smith.[35] Additionally, Mihalkovic and Widom[10] performed Ab initio calculation of enthalpies of formation of intermetallic phases at 0 K. Obtained results were in good agreement with experimental data of Subramanian and Smith.[35] Based on the first principle calculations of Mihalkovic and Widom,[10] the $Fe_{17}Y_2$ and $Fe_{23}Y_6$ phases were considered to be unstable at low temperatures. However, there is no experimental data confirming this.

First magnetic studies were carried out by Kirchmayr,[40] Kirchmayr and Steiner[41] and Besnus et al.[42] As it was mentioned above, alloys in the Fe-Y system are of interest as potential permanent magnetic materials. Therefore, many investigations of magnetic properties of intermetallic compounds of the Fe-Y system were subsequently performed. Experimental data on Curie temperature and magnetic moment are listed in the Table 2.

It should be mentioned that magnetocaloric effect in the $Fe_{17}Y_2$ compound has been studied in the work of Mandal et al.[58] Herewith, the ferromagnetic-to-paramagnetic phase transition was studied by measuring the heat capacity at constant pressure (C_P) using a PPMS device (quantum design) in the temperature range of 2-300 K.[58] However, x-ray diffraction pattern for the sample has shown deviation from literature data on crystal structure,[21,22] namely some reflections were absent in the diffraction pattern of the obtained samples. Moreover, according to Mandal et al.,[58] the magnetic transformation occurs at 295 K. This temperature significantly differs from the mean value of Curie temperature for the $Fe_{17}Y_2$ compound. A reason of this difference could be a deviation of the sample composition from nominal. The magnetocaloric effect at 295 K had a contribution in the heat capacity of samples. This can result in overestimated value for standard entropy at 298.15 K. Therefore, experimental technique of the sample preparation used by Mandal et al.[58] was not sufficient in order to obtain heat capacity data of high accuracy, which allow precise determination of the standard entropy for magnetic intermetallic compound $Fe_{17}Y_2$ at 298.15 K.

As it was said above, thermodynamic assessment of the Fe-Y system performed by Du et al.[4] suffered by several inconsistencies between experimental and calculated data for phase relations as well as for thermodynamic properties. In their work, the compound $Fe_{23}Y_6$ was formed by the peritectic reaction Liq + Fe_3Y → $Fe_{23}Y_6$ (at 1573 K) instead of its congruent melting and the eutectic reaction Liq → Fe_3Y + $Fe_{23}Y_6$ (at 1523 K). The Fe_2Y and $Fe_{23}Y_6$ compounds have been modeled as stoichiometric phases. This assessment was performed 20 years ago[4] and recent data are not accounted there. Thermodynamic assessments of Fe-Y system performed by Gong et al.[5] and then Lu et al.[7] and Kardellass et al.[8] presented only phase diagram without publishing thermodynamic parameters. Moreover, these optimizations have been carried out based on limited amount of experimental data and no comparison of calculated thermodynamic properties with available experimental results was presented. Therefore, results obtained in the works [4,5,7,8] will not be further discussed in the present paper.

In the thermodynamic assessment of the Fe-Y system performed by Kardellass et al.,[9] the excess Gibbs energy of the liquid phase has been described using a polynomial temperature dependence (PTD) in the form of $A + BT + CT^2$ and an exponential temperature dependence (ETD) of mixing parameters by Kaptay in the form of $A \cdot \exp\left(-\frac{T}{B}\right)$.[66] The CT^2 term in the PTD has been added in order to avoid the occurrence of an unwanted inverted miscibility gap in the liquid phase at high temperatures.[9] The addition of this term into the equation of the mixing parameter can be interpreted as some contribution of the excess heat capacity into the excess Gibbs energy. However, the information about excess heat capacity is not available. Optimization of excess Gibbs energy using Kaptay's ETD was used by Kardellass et al.[9] as the way to avoid the high temperature artefacts of inverted miscibility gap, caused by linear temperature dependence. In the work of Kardellass et al.,[9] it was stated, that the thermodynamic description optimized by Kaptay's ETD reproduces experimental data better than the description optimized by PTD. However, it was revealed that both thermodynamic descriptions presented by Kardellass et al.[9] gave

Table 2 Experimental data on Curie temperatures and mean magnetic moments of intermetallic compounds of the Fe-Y system

Phase	Curie temperature, K	Mean magnetic moment μ_B per Fe atom	References
$Fe_{17}Y_2$	322	…	43
	300	2.00	44
	341	2.01	45
	310	1.92	46
	328	2.20	47
	336	2.00	48
	309	1.99	49
	308	…	50
	324	2.00	51
	309	2.00	52
	327	1.78	53
	…	2.01	54, 55
	…	2.04	55, 56
	324	1.93	26
	300	1.79	57
	295	…	58
$Fe_{23}Y_6$	484	1.86	59
	490	1.88	40
	…	1.91	55, 56
	…	1.97	55, 60
	…	1.93	41, 55
	481	1.87	26
Fe_3Y	…	1.67	55, 56
	…	1.63	55, 61
	569	1.75	26
Fe_2Y	552	…	62
	545	…	63
	545	1.45	30
	534	1.44	64
	545	1.40	40
	545	1.45	65
	542	1.45	26

miscibility gap in the liquid phase at low temperatures that could cause artefacts in high-order systems. Moreover, it should be mentioned, that results calculated by Kardellass et al.[9] have significant deviations from experimental data on Gibbs energy, enthalpy and entropy of formation[35] because available data on Gibbs energy[11] and enthalpy[10] of formation were not taken into account in optimization.[9] It should be noted that the activity data obtained by vapor pressure measurements[34] indicated larger negative deviations from ideal behavior than calculated using both descriptions of Kardellass et al.[9]

In thermodynamic assessments presented by Konar et al. in the works,[12,13] the modified quasichemical model was used to describe the liquid solution. It should be also noted that homogeneity ranges in the $Fe_{23}Y_6$ and Fe_2Y indicated by Ref 14 and 17 were not taken into account by Konar et al.[12,13] The latest thermodynamic description[12] does not reproduce phase diagram better than already mentioned description.[9] The same problem to reproduce vapor pressure data[34] was found in both assessments Ref 12 and 9. It should be mentioned that the enthalpy and entropies of formation of intermetallic compounds were not well reproduced by Konar et al.[12] Because the model used by Konar et al.[12] is not compatible with the one used in the present work and taking into account the fact that that the description of the work[12] does not provide substantially better fit to experimental data than other available descriptions the results of assessment[12] will not be further discussed.

3 Thermodynamic Modeling

The thermodynamic descriptions of Gibbs energy of the pure element $i (i = \mathrm{Fe}, \mathrm{Y})$ in the Φ phase referred to the enthalpy of its phase at 298.15 K were taken from SGTE database version 5.0[67] in the following form:

$$\begin{aligned} GH\Phi_i &= {}^0G_i^{\Phi}(T) - {}^0H_i^{\Phi}(298.15\,\mathrm{K}) \\ &= a + bT + cT\ln T + dT^2 + eT^3 + fT^{-1} + gT^7 \\ &\quad + hT^{-9} \end{aligned} \qquad \text{(Eq 1)}$$

Magnetic contribution to the thermodynamic properties was taken into account according to Inden–Hillert–Jarl[68] formalism (Eq 2).

$$G_m^{\Phi,\mathrm{mag}} = RT\ln(\beta_0 + 1)g(\tau) \qquad \text{(Eq 2)}$$

where $\tau = T/T^*$, T^* is the critical temperature (the Curie temperature T_C for ferromagnetic materials or the Neel temperature T_N for antiferromagnetic materials), β_0 the average magnetic moment per atom and $g(\tau)$ is a function depending on τ.[69]

Substitutional solutions were modeled using following equation:

$$\begin{aligned} G_m^{\Phi} &= G_m^{\Phi,\mathrm{srf}} + G_m^{\Phi,\mathrm{conf}} + G_m^{\Phi,\mathrm{Ex}} \\ &= \sum_i^n x_i^0 G_i^{\emptyset} + RT\sum_i^n x_i \ln x_i + G_m^{\Phi,\mathrm{Ex}} \end{aligned} \qquad \text{(Eq 3)}$$

where $G_m^{\Phi,\mathrm{srf}} = \sum_i^n x_i^0 G_i^{\Phi}$ is the surface of reference term, $G_m^{\Phi,\mathrm{conf}} = RT\sum_i^n x_i \ln x_i$ is Gibbs free energy resulting from the configurational entropy of mixing for disorder solution, and $G_m^{\Phi,\mathrm{Ex}}$ is the excess Gibbs free energy of mixing.

The excess Gibbs free energy of mixing was modeled using Redlich–Kister polynomials,[70] expressed as:

$$G_m^{\Phi,\mathrm{Ex}} = x_A x_B \sum_{v=0}^{n} {}^vL_{A,B}^{\Phi}(x_A - x_B)^v \qquad \text{(Eq 4)}$$

The Gibbs energy $G_{A_aB_b}(T)$of a stoichiometric phase A_aB_b in case of absence of heat capacity data was modeled as:

$$G_{A_aB_b} - a \cdot {}^0H_A^{\Phi}(298.15\,\mathrm{K}) - b \cdot {}^0H_B^{\Phi}(298.15\,\mathrm{K}) = a \cdot \mathrm{GHSER}_A + b \cdot \mathrm{GHSER}_B + \alpha + \beta \cdot T \quad \text{(Eq 5)}$$

where GHSER_i is the Gibbs energy of the pure element i referred to the enthalpy of pure element i at 298.15 K in its standard element reference (SER) state, α and β are parameters to be optimized.

Homogeneity ranges of BCC, FCC and HCP phase, as well as the liquid phase were described using substitutional model with one sublattice in the form of (Fe,Y). Stable intermediate compounds in the Fe-Y system which have homogeneity ranges were described by the two-sublattice model with convenient substitution in each sublattice in form of compound energy formalism.[71] For the considered case $(\mathrm{Fe,Y})_a(\mathrm{Fe,Y})_b$, mole fraction of all end-members in the first ($y'_{\mathrm{Fe/Y}}$) and second ($y''_{\mathrm{Y/Fe}}$) sublattice must be considered in the Eq 3 as following.

$$\begin{aligned} G_m^{\Phi,\mathrm{srf}} + G_m^{\Phi,\mathrm{conf}} + G_m^{\Phi,\mathrm{Ex}} &= y'_{\mathrm{Fe}}y''_{\mathrm{Y}} \cdot {}^0G^{\Phi}_{\mathrm{Fe:Y}} + y'_{\mathrm{Fe}}y''_{\mathrm{Fe}} \cdot {}^0G^{\Phi}_{\mathrm{Fe:Fe}} \\ &\quad + y'_{\mathrm{Y}}y''_{\mathrm{Y}} \cdot {}^0G^{\Phi}_{\mathrm{Y:Y}} + y'_{\mathrm{Y}}y''_{\mathrm{Fe}} \cdot {}^0G^{\Phi}_{\mathrm{Y:Fe}} \\ &\quad + RT\left[a\left(y'_{\mathrm{Fe}}\ln\left(y'_{\mathrm{Fe}}\right) + y'_{\mathrm{Y}}\ln\left(y'_{\mathrm{Y}}\right)\right)\right. \\ &\quad \left. + b\left(y''_{\mathrm{Y}}\ln\left(y''_{\mathrm{Y}}\right) + y''_{\mathrm{Fe}}\ln\left(y''_{\mathrm{Fe}}\right)\right)\right] \\ &\quad + G_m^{\Phi,\mathrm{Ex}} {}^0G^{\Phi}_{\mathrm{Fe:Y}} = a \cdot \mathrm{GHSER}_{\mathrm{Fe}} + b \cdot \mathrm{GHSER}_Y \\ &\quad + \alpha + \beta \cdot T {}^0G^{\Phi}_{\mathrm{Fe:Fe}} = (a+b) \cdot \mathrm{GHSER}_{\mathrm{Fe}} \\ &\quad + \gamma {}^0G^{\Phi}_{\mathrm{Y:Y}} = (a+b) \cdot \mathrm{GHSER}_{\mathrm{Y}} + \sigma {}^0G^{\Phi}_{\mathrm{Y:Fe}} \\ &= a \cdot \mathrm{GHSER}_Y + b \cdot \mathrm{GHSER}_{\mathrm{Fe}} - \alpha - \beta \cdot T \\ &\quad + \gamma + \sigma \end{aligned} \quad \text{(Eq 6)}$$

In the frame of the present work, the excess energy contribution $G_m^{\Phi,\mathrm{Ex}}$ was zero, as mixing parameters ${}^0L^{\Phi}_{\mathrm{Fe,Y:Y}} = {}^0L^{\Phi}_{\mathrm{Fe,Y:Fe}}$ and ${}^0L^{\Phi}_{\mathrm{Fe:Y,Fe}} = {}^0L^{\Phi}_{\mathrm{Y:Y,Fe}}$ were stated to be zero.

The assessment of thermodynamic parameters and phase diagram calculations of the Fe-Y system were performed using Thermo-Calc program set using correspondently PARROT module and POLY-3 module.[72,73]

4 Optimization Strategy

At the first step of the optimization procedure, intermetallic compounds Fe_2Y and $Fe_{23}Y_6$ with homogeneity ranges were accepted to be stoichiometric. Then, they were treated using a two-sublattice model with convenient substitution in each sublattice: $(\mathrm{Fe,Y})_2(\mathrm{Y,Fe})$ and $(\mathrm{Fe,Y})_{23}(\mathrm{Y,Fe})_6$ respectively.

The substitutional model was accepted to describe the liquid phase. The binary interaction parameters of ${}^{\upsilon}L^{\emptyset}_{A,B}$ were assessed in the present work using the linear temperature dependence $A - B \cdot T$. According to this equation, the enthalpy of mixing and the excess entropy of mixing related to the constant parameters A and B, respectively. According to Kaptay, this is a very rough assumption.[66] Generally, if B has negative sign then the excess Gibbs energy at mid-composition grows positively with the temperature. This results in an inverted miscibility gap with a lower critical temperature of $T_{\mathrm{c,min}} = A/(B + 2R)$[66] (where R is the gas constant). However, according to Schmid-Fetzer et al.,[74] it does not contradict with the fact that real systems exist at temperatures lower than critical temperature and de-mixing occurs over some very high temperature range. Therefore, the linear temperature dependence can be used in the defined temperature interval up to $T_{\mathrm{c,min}}$.

Kaptay[66] suggested a possibility of trying to avoid the artificial miscibility gap completely, by bringing liquid excess parameters to zero at high temperatures using an exponential function of the following form:

$${}^{\upsilon}L^{\mathrm{Liq}}_{A,B} = h_0 \exp\left(-\frac{T}{\tau_0}\right) \quad \text{(Eq 7)}$$

where h_0 and τ_0 are the two adjustable parameters

Schmid-Fetzer et al.[74] have mentioned, that Kaptay's model allows avoiding the inverted gap, while other artifacts at low temperature can be observed. In the case of the negative enthalpy of mixing in liquid alloys, one parameter must have $h_0 < 0$, resulting in negative excess Gibbs energy. The exponential function, however, exaggerates this negative excess Gibbs energy at very low temperature, resulting in the re-stabilization of the liquid phase way below the solidus. Later, Kaptay revised the exponential excess Gibbs energy model in to the form of the combined linear-exponential model.[75] He stated that the combined linear-exponential model should be used instead of the exponential model in the case of occurring of artifacts at low temperatures. However, the application of such complex models to describe the excess Gibbs energy can be unreasonable. Therefore, linear temperature dependence was applied in the present work to assess binary interaction parameters of ${}^{\upsilon}L^{\emptyset}_{A,B}$ with special care to avoid a miscibility gap at high temperatures.

In order to decrease deviation between calculated and experimental data, method of least squares has been used with help of the PARROT module of Thermo-Calc. Individual weights have been predetermined for every type of experimental data considering possible deviation and accuracy of the each experimental method. As it was said above, a contribution of heat capacity into the enthalpy of formation have not been considered (i.e. $\Delta C_p =$

0 in the range between 0 and 298.15 K). Therefore, results of ab-initio calculations of enthalpies of formation of intermetallic compounds were taken into account as enthalpies of formation at 298.15 K. It should be mentioned that the results of Sudavtsova et al.[33] were not used in optimization because they are obtained in the narrow range of compositions deviation from accepted data of Ryss et al.[32]

Increasing of number of excess interaction parameters and complication of their temperature dependence description do not always lead to the best accordance between experimental data and calculated results. Therefore, optimization strategy was aimed to get the best agreement of the thermodynamic description with collected literature data on phase relations and thermodynamic properties using a minimum of parameters. The general "χ^2"–criterion (Eq 8)[76] has been used during the optimization process as a method to compare current in the present work and published earlier thermodynamic descriptions considering its number of independent optimized parameters.

$$\chi^2 = \sum_{i=1}^{N} \left[\frac{\alpha_{i.\text{cal.}} - \alpha_{i.\text{exp.}}}{\delta\alpha_{i.\text{exp.}}} \right]^2 \cdot (N - p - 1)^{-1} \qquad \text{(Eq 8)}$$

where $\alpha_{i.\text{exp.}}$ an experimental value with an error $\delta\alpha_{i.\text{exp.}}$; $\alpha_{i.\text{cal.}}$ a calculated value of a thermodynamic description; p a number of independent optimized parameters; N a general number of experimental values.

The $Fe_{17}Y_2$ phase was described without the high temperature modification because of an insufficiency of experimental information. Experimental results of invariant reactions and phase relations had the most weight during the optimization of thermodynamic parameters of the Fe-Y system. Average values of experimental Curie temperature and mean magnetic moment of intermetallic compounds were used in order to consider the magnetic contribution to the thermodynamic properties. The Curie temperature and mean magnetic moment for FCC and BCC phases were taken according to SGTE database version 5.0.[67]

5 Results and Discussion

Optimized thermodynamic parameters of the obtained thermodynamic description are listed in the Table 3. The calculated Fe-Y phase diagram is presented in the Fig. 2 along with experimental data. Comparison of calculated invariant reactions with experimental data and results obtained in the previous thermodynamic assessment[9] are presented in the Table 4. It should be mentioned, that methods used by Domagala et al.[14] to determine solidus lines of the diagram were based on the optical determination of visible melting. Therefore, that experimental data obtained in the work of Domagala et al.[14] had significant uncertainty. The most accurate temperature was stated for eutectic reaction Liq $\leftrightarrow Fe_2Y + \alpha$ Y with an error of ± 10 K. Temperature deviations of eutectic Liq $\leftrightarrow \gamma$ Fe + $Fe_{17}Y_2$, congruent Liq $\leftrightarrow Fe_{17}Y_2$ and peritectic Liq + $Fe_3Y \leftrightarrow Fe_2Y$ reactions were given as ± 25 K. Other temperatures were denoted as rough values. The error of these values can be estimated to be about ± 50 K. An accuracy of the published values on chemical compositions of the liquid phase was given to be about 0.1 at.% for all invariant reactions. However, considering investigation methods used by Domagala et al.,[14] it can be stated, that obtained experimental results of chemical compositions of invariant reactions cannot be defined more accurately than ± 1 at.%. It must be mentioned, that the chemical composition of liquid in the peritectic reaction Liq + $Fe_3Y \leftrightarrow Fe_2Y$ has been denoted as a rough value. Therefore, it can be concluded, that good agreement of calculated results with experimental data on phase relations within error ranges was achieved.

Figure 3 shows the integral enthalpy of mixing of the liquid phase versus the mole fraction of yttrium at temperature of 1873 K calculated in the present work and in the work of Kardellass et al.[9] in comparison with experimental data of Ryss et al.[32] The reference state of both elements was accepted as liquid at 1873 K. The calculated curve had a minimum value of -7.96 kJ mol^{-1} 47 at.% Y, which perfectly agrees with experimental value of -8.44 kJ mol^{-1} obtained for the same composition.[32] It is clearly evident that the calculated results obtained in the present work have reproduced the experimental data better than in the work of Kardellass et al.[9] The maximal deviation is $\sim 5\%$.

Figure 4 presents the activities of iron and yttrium calculated data of this work compared to the measured ones using Knudsen effusion mass spectrometry (KEMS) by Nagai et al.[34] The activities were found to be inconsistent with calculations of the present work, especially activity of iron. According to the experimental results, activities of iron and yttrium should have large negative deviation from ideal behavior. In the present optimization less negative deviation from ideal behavior in liquid phase than obtained by [34] is required in order to reproduce the phase diagram (see Fig. 1), as well as experimental data on the Gibbs energy, enthalpy and entropy of formation of intermetallic compounds obtained in the works.[10,11,35] Using obtained values a_{Fe} and a_Y, Nagai et al.[34] determined the temperature dependence of the Gibbs energy of formation of Fe_3Y to be $(-29.75 + 8.5 \cdot 10^{-3} \cdot T(K))$ kJ mol^{-1}. Obtained result considerably differs from values obtained in other works.[10,11,35] Consequently, it can be concluded, that

Table 3 Optimized thermodynamic parameters of the Fe-Y system (J mol^{-1})

Phase	Sublattice model	Optimized parameters
Liq	$(Fe, Y)_1$	${}^0L^{Liq}_{Fe,Y} = -31714.1 + 17 * T$
		${}^1L^{Liq}_{Fe,Y} = -3806.7$
FCC_A1	$(Fe, Y)_1$	${}^0L^{FCC\_A1}_{Fe,Y} = +50000$
HCP_A3	$(Fe, Y)_1$	${}^0L^{HCP\_A3}_{Fe,Y} = +34000$
BCC_A2	$(Fe, Y)_1$	${}^0L^{BCC\_A2}_{Fe,Y} = +54000$
$Fe_{17}Y_2$	$(Fe)_{17}(Y)_2$	${}^0G^{Fe17Y2}_{Fe:Y} - 17*{}^{298.15}H^{BCC\_A2}_{Fe} - 2*{}^{298.15}H^{HCP\_A3}_{Y} = +17$*GHSERFE + 2*GHSERY − 237121 + 97 * T
		${}^{298.15}TC^{Fe17Y2}_{Fe:Y} = 318$
		${}^{298.15}Bmag^{Fe17Y2}_{Fe:Y} = 1.98$
$Fe_{23}Y_6$	$(Fe, Y)_{23}(Y, Fe)_6$	${}^0G^{Fe23Y6}_{Fe:Y} - 23*{}^{298.15}H^{BCC\_A2}_{Fe} - 6*{}^{298.15}H^{HCP\_A3}_{Y} =$ +23*GHSERFE + 6*GHSERY − 389791 + 131 * T
		${}^0G^{Fe23Y6}_{Fe:Fe} - 29*{}^{298.15}H^{BCC\_A2}_{Fe} = +29$*GHSERFE + 190000
		${}^0G^{Fe23Y6}_{Y:Y} - 29*{}^{298.15}H^{HCP\_A3}_{Y} = +29$*GHSERY + 650000
		${}^0G^{Fe23Y6}_{Y:Fe} - 6*{}^{298.15}H^{BCC\_A2}_{Fe} - 23*{}^{298.15}H^{HCP\_A3}_{Y} = +6$*GHSERFE + 23*GHSERY + 389791 − 131 * T + 840000
		${}^{298.15}TC^{Fe23Y6}_{Fe:Y} = 483$
		${}^{298.15}Bmag^{Fe23Y6}_{Fe:Y} = 1.75$
Fe_3Y	$(Fe)_3(Y)$	${}^0G^{Fe3Y}_{Fe:Y} - 3*{}^{298.15}H^{BCC\_A2}_{Fe} - {}^{298.15}H^{HCP\_A3}_{Y} = +3$*GHSERFE + GHSERY − 51446 + 14 * T
		${}^{298.15}TC^{Fe3Y}_{Fe:Y} = 539$
		${}^{298.15}Bmag^{Fe3Y}_{Fe:Y} = 1.65$
Fe_2Y	$(Fe, Y)_2(Y, Fe)$	${}^0G^{Fe23Y6}_{Fe:Y} - 2*{}^{298.15}H^{BCC\_A2}_{Fe} - {}^{298.15}H^{HCP\_A3}_{Y} = +2$*GHSERFE + GHSERY − 33886 + 8 * T
		${}^0G^{Fe23Y6}_{Fe:Fe} - 3*{}^{298.15}H^{BCC\_A2}_{Fe} = +3$*GHSERFE + 30,000
		${}^0G^{Fe23Y6}_{Y:Y} - 3*{}^{298.15}H^{HCP\_A3}_{Y} = +3$*GHSERY + 100,000
		${}^0G^{Fe23Y6}_{Y:Fe} - {}^{298.15}H^{BCC_A2}_{Fe} - 2*{}^{298.15}H^{HCP_A3}_{Y} = +$GHSERFE + 2*GHSERY + 33,886 − 8 * T + 130000
		${}^{298.15}TC^{Fe2Y}_{Fe:Y} = 544$
		${}^{298.15}Bmag^{Fe2Y}_{Fe:Y} = 1.45$

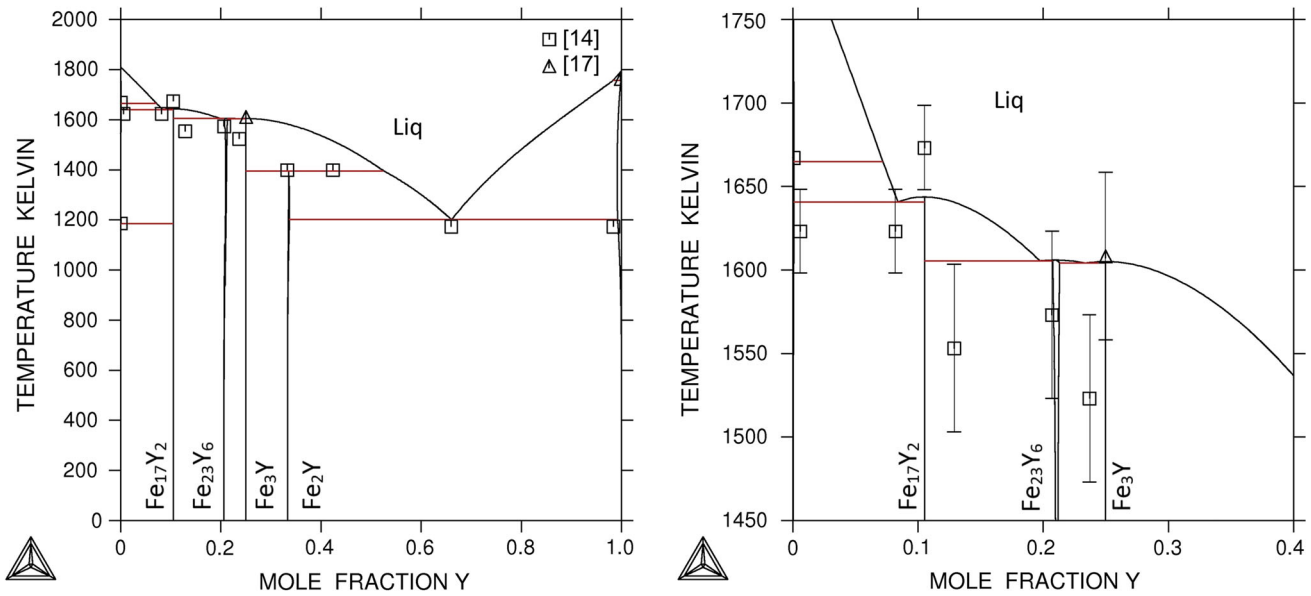

Fig. 2 Calculated Fe-Y phase diagram with experimental data[14,17]

obtained experimental information and activity data by Nagai et al.[34] are inconsistent. Similar inconsistencies were observed for the database of Kardellass et al.[9] It should be mentioned the substantial inconsistencies were also observed for the calculations in the system of Fe-La[77] in comparison with experimental data of Nagai et al.[34] According to Konar et al.,[77] a reason of the inconsistencies could be a significant error in ion current measurements in the KEMS.

The Gibbs energy, enthalpy and entropy of formation calculated in the present work are compared with experimental data and calculations of Kardellass et al.[9] are listed in the Table 5. It can be seen that there is reasonable agreement between calculated and experimental results for the Gibbs energy, enthalpy and entropy of formation. It should be mentioned, that the $Fe_{17}Y_2$ and $Fe_{23}Y_6$ compounds were stated to be unstable at 0 K based on the results of Ab-initio calculations of Mihalkovic and Widom. Nevertheless, there are no experimental data about any phase transformation in the Fe-Y binary system at low temperatures. Additionally, it should be noted, that these results of first principle calculations had minor statistical weight during the optimization process in comparison with experimental data. However, as it can be seen in the Table 5, there is acceptable accordance between Ab-inition results and values calculated in this work. The Gibbs energy and enthalpy of formation calculated using the thermodynamic description of the present work are compared with experimental data of Subramanian and Smith[35] and calculations of Kardellass et al.[9] in the Fig. 5.

Based on the experimental results of heat capacity measurement performed by Mandal et al.,[58] the standard entropy at 298.15 K of the $Fe_{17}Y_2$ compound have been calculated equal to 34.5 J K^{-1} mol^{-1} in the present work. As mentioned above, the technique of the sample preparation used in the work of Mandal et al.[58] does not allow high accuracy calculation of the standard entropy. However, the agreement between the value calculated based on C_p data of Mandal et al.[58] and value derived in the present optimization is quite acceptable (compare value of 34.5 J K^{-1} mol^{-1} based on data of Mandal et al.[58] with 32.4 J K^{-1} mol^{-1} calculated using present thermodynamic description).

All available experimental and theoretical results including information that was not considered earlier[10,11] were taken into account during the optimization of present thermodynamic description. The "χ^2"-criterion (see Eq 8) was calculated for the present optimization and for available in the literature thermodynamic descriptions.[9] Evaluated results of the work of Kardellass et al.[9] were the following: $\chi^2 = 2131.0$ for PTD ($\chi^2_{inv.} = 2.4$ considering only experimental data on invariant reactions, the number of independent optimized parameters $p = 25$) and $\chi^2 = 986.3$ for ETD ($\chi^2_{inv.} = 2.9$, $p = 27$). Calculated result of current optimization was $\chi^2 = 497.0$ ($\chi^2_{inv.} = 1.0$, $p = 18$). Calculation of the "χ^2"-criterion for each

Table 4 Invariant reactions in the Fe-Y system: comparison between experimental data,[14,17,31,69] calculation of Kardellass et al.[9] and current results

Reaction	Type	Temperature, K	Phase composition (Y, at.%)			Source
Liq + δ Fe ↔ γ Fe	Metatectic	1665	…	…	…	Ref 17, 69
		1665	7.19	…	…	This work
		1663	4.79	…	…	PTD[9]
		1664	4.79	…	…	ETD[9]
γ Fe ↔ α Fe + $Fe_{17}Y_2$	Peritectoid	1184	…	0.038	10.50	Ref 17, 31, 69
		1185	…	0.001	10.50	This work
		1185	…	…	10.50	PTD[9]
		1185	…	…	10.50	ETD[9]
Liq ↔ δ Fe + $Fe_{17}Y_2$	Eutectic	1663	7.19	…	10.50	ETD[9]
Liq ↔ γ Fe + $Fe_{17}Y_2$	Eutectic	1623 ± 25	8.20	<0.60	10.50	Ref 14, 17
		1641	8.41	0.10	10.50	This work
		1633	5.63	…	10.50	PTD[9]
Liq ↔ $Fe_{17}Y_2$	Congruent	1673 ± 25	10.50	10.50	…	Ref 14, 17
		1644	10.50	10.50	…	This work
		1676	10.50	10.50	…	PTD[9]
		1672	10.50	10.50	…	ETD[9]
Liq ↔ $Fe_{17}Y_2$ + $Fe_{23}Y_6$	Eutectic	~1553	12.90	10.50	…	Ref 14, 17
		1605	19.74	10.50	20.70	This work
		1605	18.15	10.50	…	PTD[9]
		1638	17.90	10.50	…	ETD[9]
Liq ↔ $Fe_{23}Y_6$	Congruent	~1573	…	…	…	Ref 14, 17
		1606	20.05	20.05	…	This work
		1606	20.75	20.75	…	PTD[9]
		1641	20.75	20.75	…	ETD[9]
Liq ↔ $Fe_{23}Y_6$ + Fe_3Y	Eutectic	~1523	23.70	…	25	Ref 14, 17
		1604	23.36	20.50	25	This work
		1605	20.70	…	25	PTD[9]
		1640	21.63	…	25	ETD[9]
Liq ↔ Fe_3Y	Congruent	~1608	25	25	…	Ref 14, 17
		1605	25	25	…	This work
		1623	25	25	…	PTD[9]
		1647	25	25	…	ETD[9]
Liq + Fe_3Y ↔ Fe_2Y	Peritectic	1398 ± 25	~42	25	33.30	Ref 14, 17
		1396	52.48	25	33.54	This work
		1409	44.27	25	33.30	PTD[9]
		1397	48.18	25	33.30	ETD[9]
Liq ↔ Fe_2Y + α Y	Eutectic	1173 ± 10	~66	~33.3	>98.40	Ref 14, 17
		1201	66.09	33.7	99.20	This work
		1146	61.18	…	…	PTD[9]
		1118	63.65	…	…	ETD[9]
Liq + β Y ↔ α Y	Peritectic	1758	…	…	…	Ref 69
		1756	98.26	99.74	99.73	This work
		1750	97.89	…	…	PTD[9]
		1749	97.60	…	…	ETD[9]

thermodynamic description considered an identical number of experimental values of reliable literature data (85 experimental values including 16 points of phase equilibria). Errors of experimental values were taken according to their accuracy. It can be concluded, that thermodynamic description derived in the present work

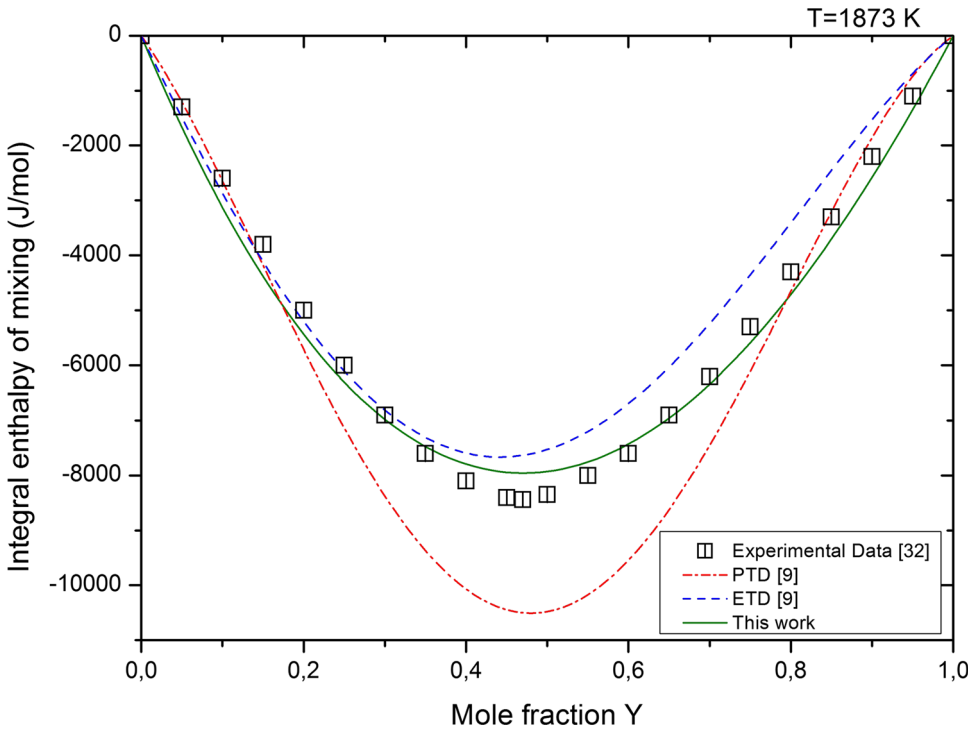

Fig. 3 Comparison of integral mixing enthalpies of liquid phase obtained in the present work (solid green line) and in the work of Kardellass et al.[9] using polynomial temperature dependence of interaction parameters description (PTD, dash-dot red line) and exponential temperature dependence of Kaptay[66] (EDT, dashed blue line) together with experimental results of Ryss et al.[32]

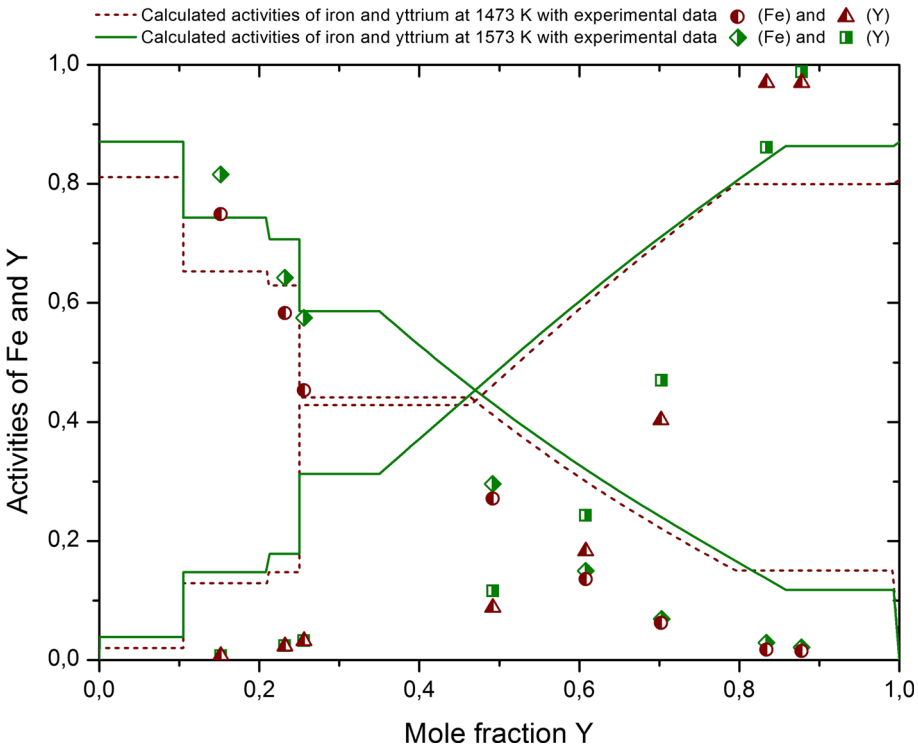

Fig. 4 Comparison of our calculated data and the experimental results of activities from the work of Nagai et al.[34]

describes experimental data better than thermodynamic descriptions published earlier. Moreover, the number of optimized thermodynamic parameters in the present work was less than in previous assessments. Optimized parameters describing excess mixing energy of liquid phase do not lead to miscibility gap in the liquid phase in the whole range of temperatures of SGTE functions of pure elements. Therefore, obtained thermodynamic description is acceptable for the modeling of the high-order systems.

Table 5 Comparison of the experimental and calculated data on Gibbs energy, enthalpy and entropy of formation of intermetallic compounds of the Fe-Y system

Intermetallic compounds	Temperature, K	Enthalpy of formation, kJ (mol at)$^{-1}$	Entropy of formation, kJ^{-1} (mol at)$^{-1}$	Gibbs energy of formation, kJ (mol at)$^{-1}$	Used method	References
$Fe_{17}Y_2$	0	−1.78*			Ab initio	Ref 10
	298.15	−8.7			Prediction (a)	Ref 11
		−4.36			Optimization	This work
		−5.99			Optimization	PTD[9]
		−5.29			Optimization	ETD[9]
	895	−7.93 ± 0.01	−1.72 ± 0.02	−4.6 ± 0.6	EMF	Ref 11
		−6.66	−1.74	−6.72	Optimization	This work
		−8.35	2.838	−10.89	Optimization	PTD[9]
		−7.66	1.015	−8.57	Optimization	ETD[9]
	973	−6.38 ± 0.31	−1.90 ± 0.28	−4.54 ± 0.05	EMF	Ref 35
		−7.77	−1.121	−6.68	Optimization	This work
		−9.47	1.660	−11.09	Optimization	PTD[9]
		−8.76	−0.167	−8.60	Optimization	ETD[9]
$Fe_{23}Y_6$	0	−4.85*			Ab initio	Ref 10
	298.15	−6.25			Optimization	This work
		−12.05			Optimization	PTD[9]
		−12.97			Optimization	ETD[9]
	973	−8.09 ± 0.49	−2.24 ± 0.44	−5.91 ± 0.07	EMF	Ref 35
		−9.22	−0.933	−8.31	Optimization	This work
		−11.69	2.970	−14.58	Optimization	PTD[9]
		−12.65	−0.079	−12.57	Optimization	ETD[9]
Fe_3Y	0	−7.60			Ab initio	Ref 10
	298.15	−1			Prediction (a)	Ref 39
		−6.96			Optimization	This work
		−13.04			Optimization	PTD[9]
		−13.31			Optimization	ETD[9]
	973	−8.97 ± 0.54	−3.03 ± 0.48	−6.02 ± 0.08	EMF	Ref 35
		−8.94	−0.184	−8.76	Optimization	This work
		−12.49	3.570	−15.96	Optimization	PTD[9]
		−12.77	0.859	−13.61	Optimization	ETD[9]
Fe_2Y	0	−7.87			Ab initio	Ref 10
	298.15	−1			Prediction (a)	Ref 39
		−6.3			Optimization	This work
		−9.99			Optimization	PTD[9]
		−12.47			Optimization	ETD[9]
	973	−7.09 ± 0.61	−0.96 ± 0.55	−6.15 ± 0.09	EMF	Ref 35
		−7.77	0.32	−8.09	Optimization	This work
		−12.55	2.87	−15.34	Optimization	PTD[9]
		−11.80	1.14	−12.91	Optimization	ETD[9]
FeY	0	−5.9			Interpolation	Ref 10
	298.15	−2			Prediction (a)	Ref 39
		−12.5			Prediction (b)	Ref 37
	973	−5.3		−4.6	Interpolation	Ref 35
		−5.8		−6.0	Interpolation	This work
		−9.4		−11.5	Interpolation	PTD[9]
		−8.8		−9.7	Interpolation	ETD[9]

(a)Using the Miedema theory

(b)Using Friedel-type d-band model

* These compounds are unstable at 0 *K* according to the ab initio calculation performed in the work[10]

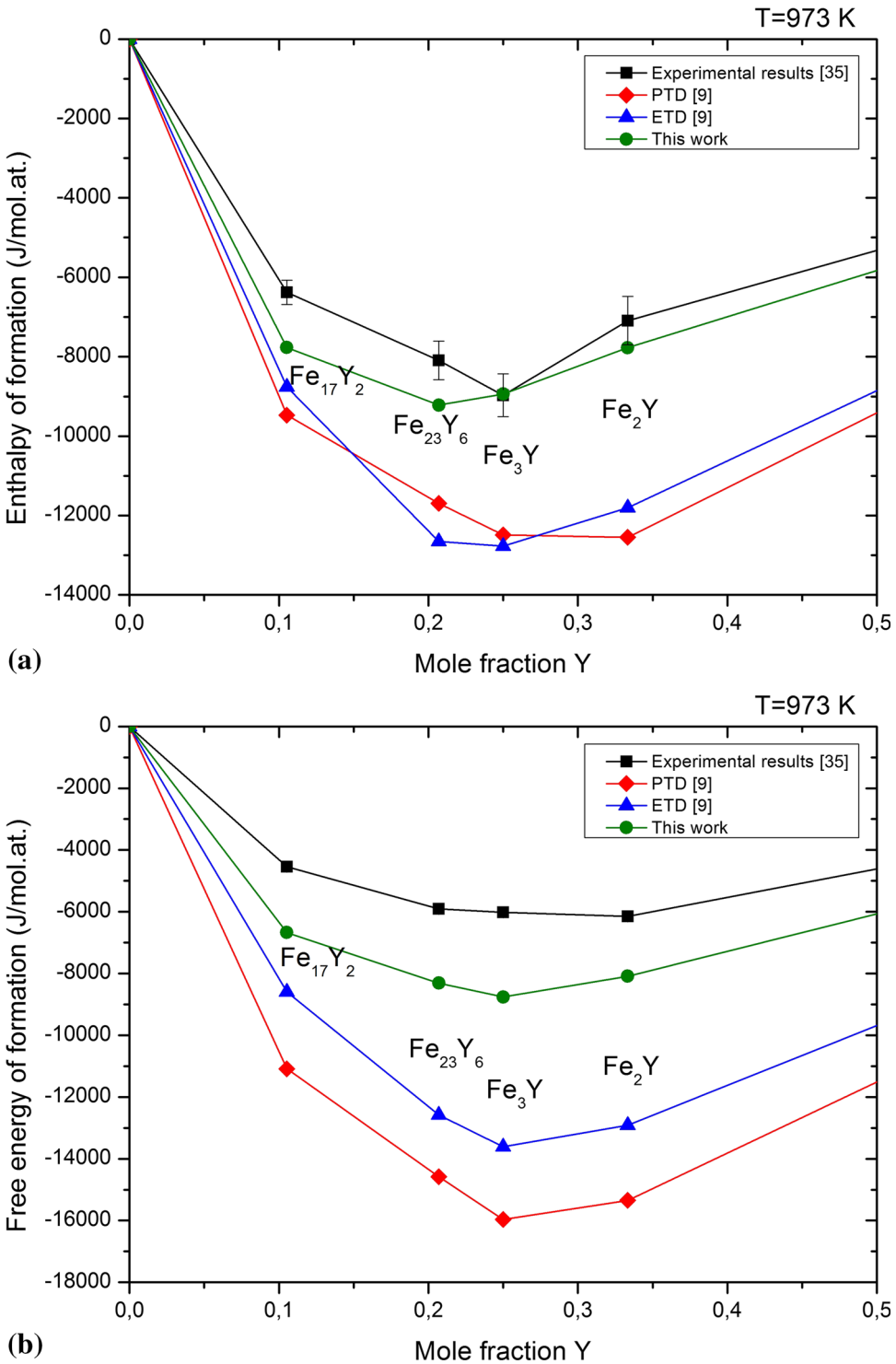

Fig. 5 (a) Comparison of the formation enthalpy of intermetallic compounds obtained in the present work (green circles) and in the work of Kardellass et al.[9] using polynomial temperature dependence of interaction parameters description (PTD, red diamonds) and exponential temperature dependence of Kaptay[66] (EDT, blue triangles) with experimental data of Subramanian and Smith[35] (black squares) and (b) Comparison of the Gibbs formation energies of intermetallic compounds calculated in the present work (green circles) and in the work of Kardellass et al.[9] using polynomial temperature dependence of interaction parameters description (PTD, red diamonds) and exponential temperature dependence of Kaptay[66] (EDT, blue triangles) with experimental data of Subramanian and Smith[35] (black squares)

6 Conclusions

Critical evaluation and optimization of all available experimental data for the Fe-Y system have been performed in order to derive a consistent set of the Gibbs energies for all the phases in the system. Available data for intermetallic compounds, namely the experimental Gibbs energy of formation[11] and ab-initio calculations of enthalpy of formation[10] have been taken into account. Liquid and solid solution phases such as bcc, fcc, and hcp have been described using substitutional model. Compound energy formalism[71] has been applied in order to describe intermetallic compounds with homogeneity range. The magnetic properties of solid phases have been taken into account. Problems of thermodynamic modelling in this system have been discussed, namely choosing, application and possible artifacts of the excess Gibbs energy descriptions. The general "χ^2"-criterion (Eq 8) has been used as a method of comparison of thermodynamic descriptions considering general number of optimized parameters. In the results, it has been established that the set of thermodynamic parameters derived in the present work describes experimental data better than thermodynamic descriptions published earlier. The calculated diagram of the Fe-Y system reproduce experimental data on phase equilibria within uncertainty. Current calculation have acceptable agreement with experimental data on the Gibbs energy, enthalpy and entropy of formation of intermetallic compound,[10,11,35] which are in good accordance with each other. Experimental data on activities[34] are inconsistent with the present thermodynamic description. However, values of Gibbs energy of formation calculated by Nagai et al.[34] using obtained data on activities are in significant inconsistence with other experimental data.[10,11,35] Considering this well accordance of the works,[10,11,35] experimental data obtained in these works have been accepted as more reliable. New activity measurements for liquid phase in this system could help to clarify the inconsistence between data and improve thermodynamic description of the Fe-Y system.

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