

THERMODYNAMIC MODELING OF THE In–Sc AND In–Y SYSTEMS SUPPORTED BY FIRST-PRINCIPLES CALCULATIONS

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Abstract

Based on an assessment of the phase equilibria and thermodynamic data in the literature, the thermodynamic modeling of the In–Sc and In–Y systems was carried out by means of the calculation of phase diagram (CALPHAD) method supported by first-principles calculations. The solution phases, i.e., liquid, (In), (α Sc), (β Sc), (α Y) and (β Y), were modeled with the substitutional regular solution model. Ten intermetallic compounds, including InSc_3 , InSc_2 , In_4Sc_3 , InSc , In_2Sc , In_3Sc , InY_2 , InY , In_3Y_3 , and In_3Y were described as stoichiometric phases, while In_3Y_3 was modeled with a sublattice model with respect to its homogeneity range. The enthalpies of formation of the intermetallic compounds at 0 K were computed using first-principle calculations and were used as input for the thermodynamic optimization. A set of self-consistent thermodynamic parameters for both the In–Sc and In–Y systems were obtained and the calculated phase diagrams are in good agreement with the experimental data.

Keywords: In–Sc; In–Y; Thermodynamic optimization; First-principles calculation; CALPHAD; Phase diagram

1. Introduction

Light alloys, like aluminum and magnesium alloys, have witnessed a huge number of applications in aviation, aerospace and automotive industry in recent years [1-3]. It is found that indium, yttrium, and scandium can be used as trace addition elements to improve the alloys' properties [4-9]. The addition of In in Mg-based alloys induces grain size refinement and precipitation hardening, thereby enhancing their mechanical properties [4, 5]. The introduction of Sc cannot only increase the yield and tensile strength but also results in a reduction in weld and solidification cracking for both Al and Mg alloys [6, 7]. Y addition refines the grain size of the alloys, leading to higher strength and better ductility [8, 9]. An alloy's property can be understood by its microstructures and it is critical to know the effect of addition elements on its phase formation and phase stability. For establishing the thermodynamic database of the Al and Mg alloys, the thermodynamic description of the In–Sc–Y system is of great interest. Because the thermodynamic descriptions of In–Sc and In–Y systems are not available in the literature, it is our goal to develop a set of sound thermodynamic parameters for these systems by means of the CALPHAD method.

2. Literature review

2.1 The In–Sc system

Using differential thermal analysis (DTA), metallography and X-ray diffraction (XRD), Yatsenko [10] constructed the first the In–Sc phase diagram. As shown in Table 1, six intermetallic compounds were reported. Among them, InSc_3 , In_3Sc_5 , InSc , In_3Sc_3 and In_3Sc decompose in peritectic reactions at 1340 °C, 1330 °C, 1120 °C, 950 °C and 910 °C respectively, while InSc_2 melts at 1420 °C congruently [10].

Palenzona et al. [18] reinvestigated the In–Sc system from 30 to 100 at.% In by means of electron microscopy, DTA, XRD, and metallographic analysis. The existence of In_3Sc , InSc_2 , and InSc_3 was confirmed. Although In_3Sc_3 and In_3Sc_5 were reported by Yatsenko [10], they were not observed by Palenzona et al. [18]. Instead, three new compounds were found, among which were one at 45 at.% In (CsCl type), one at 50 at.% In (AuCu type) and one (named as In_2Sc) at 66.67 at.% In. The first two new compounds were designated as InSc by Palenzona et al. [18]. Okamoto [19] reassessed all the phase equilibria information [10, 18], in which the work by Palenzona et al. [18] was accepted and the compound at 45 at.% In was named as In_4Sc_5 .

The crystal structure information of the stable phases in the In–Sc system is summarized in Table 1.

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Table 1. Crystal structure data of intermetallic compounds in the In–Sc and In–Y systems, together with the lattice parameters obtained by the present first-principles calculations

System	Phase	Structure Type/Pearson symbol/Space group	Lattice parameter (Å)			Reference
			a	b	c	
In–Sc	(In)	tetragonal $tI2$ $I4/mmm$	3.253		4.949	[17]
			3.263		5.17	This work
			0.31%		4.47%	Error
	(αSc)	hcp $hP2$ $P6_3/mmc$	3.304		5.225	[20]
			3.311		5.157	This work
			0.20%		1.30%	Error
	(βSc)	bcc $cI2$ $Im\bar{3}m$	3.757			[21]
			3.658			This work
			2.60%			Error
	InSc ₃	Mg ₃ Cd $hP8$ $P6_3/mmc$	6.421		5.183	[22]
			6.405		5.17	This work
			0.24%		0.25%	Error
	InSc ₂	Ni ₂ In $hP6$ $P6_3/mmc$	5.024		6.276	[18]
			5.04		6.275	This work
			0.32%		0.01%	Error
	In ₄ Sc ₅	CsCl $cP2$ $Pm\bar{3}m$	3.565			[18,19]
	InSc	AuCu $tP4$ $P4/mmm$	4.539		4.326	[18]
			4.552		4.338	This work
			0.29%		0.28%	Error
	In ₂ Sc	ZrGa ₂ $oC12$ $Cmmm$	4.44	13.571	4.459	[18]
			4.471	13.666	4.49	This work
			0.70%	0.70%	0.70%	Error
	In ₃ Sc	AuCu ₃ $cP4$ $Pm\bar{3}m$	4.479			[18]
			4.532			This work
			1.18%			Error
In–Y	(αY)	hcp $hP2$ $P6_3/mmc$	3.647		5.731	[16]
			3.596		5.707	This work
			1.40%		0.42%	Error
	(βY)	bcc $cI2$ $Im\bar{3}m$	3.967			This work
			5.37		6.79	[10]
			5.379		6.795	This work
	InY ₂	Ni ₂ In $hP6$ $P6_3/mmc$	0.16%		0.07%	Error
			5.365		6.778	[11]
			8.96		6.71	[10]
	In ₃ Y ₅	Mn ₅ Si ₃ $hP16$ $P6_3/mcm$	8.984		6.728	This work
			0.26%		0.27%	Error
			8.971		6.745	[12]
	InY	CsCl $cP2$ $Pm\bar{3}m$	3.81			[10]
			3.757			This work
			1.39%			Error
	In ₅ Y ₃	Pu ₃ Pd ₅ $oC32$ $Cmcm$	3.806			[13]
			9.87	8.1	10.3	[10]
			9.917	8.065	10.396	This work
	In ₃ Y	AuCu ₃ $cP4$ $Pm\bar{3}m$	0.05%	0.43%	0.93%	Error
			9.88	8.04	10.29	[14]
			4.6			[10]
	In ₃ Y	AuCu ₃ $cP4$ $Pm\bar{3}m$	4.642			This work
			0.91%			Error
			4.585			[15]

2.2 The In–Y system

The only experimental phase diagram on the In–Y system was investigated by Yatsenko [10] using XRD, metallography analysis, and DTA. Five intermetallic compounds, InY₂, In₃Y₅, InY, In₅Y₃, and In₃Y, were

found. Among them, In₃Y₅, In₅Y₃, and In₃Y melt congruently at 1340 °C, 1140 °C and 1110 °C, respectively. In₃Y₅ was found to have a homogeneity range of 55–56 at.% In at 1125°C. InY₂ and InY are formed in peritectic reactions at 1330 °C and 1220 °C, respectively. Four eutectic reactions, Liquid ↔ (βY) +



InY_2 , Liquid $\leftrightarrow$ InY + In_5Y_3 , Liquid $\leftrightarrow$ In_5Y_3 + In_3Y and Liquid $\leftrightarrow$ In_3Y + (In), occur at 1060 °C, 1090 °C, 1080 °C and 160 °C, respectively. A eutectoid reaction Liquid $\leftrightarrow$ (βY) + InY_2 at 1030 °C has been reported. No other experimental work is available in the literature and the phase equilibria data in Ref. [10] were adopted in the present work.

The crystal structure information of the stable phases in the In–Y system is summarized in Table 1.

3. Enthalpies of formation calculated using the first-principles calculations

It is found that the density functional theory (DFT) based first-principles calculations can provide helpful thermodynamic data that are not available in the literature or are unsuitable for its experimental operation [23–34].

In this work, the first-principles calculations were conducted within the generalized gradient approximation (GGA) [35] suggested by Perdew et al. [36] for the exchange and correlation contributions and with projector augmented plane-wave (PAW) potentials [37] for valence electrons, as implemented in the Vienna *ab initio* simulation package (VASP) [38]. The atoms were relaxed toward equilibrium until the Hellman-Feynman forces were less than $10^{-2}\text{eV}/\text{\AA}$. Brillouin-zone integrations were performed using a Monkhorst-Pack mesh [39]. The energy cut off at 400 eV was sufficient to ensure the total energy difference less than 1meV/atom. The k-points meshes for Brillouin zone sampling were constructed using Monkhorst-Pack scheme and at least 10000 per reciprocal atom were employed. The structures were fully relaxed using the Methfessel-Paxton method [40] and a final self-consistent static calculation via the tetrahedron method with Blochl corrections [41] was performed. The enthalpies of formation of the compound In_mX_n ($X=\text{Sc}$ or Y) at 0 K can be defined as the following equation:

$$\Delta H_f(\text{In}_m\text{X}_n) = E(\text{In}_m\text{X}_n) - mE(\text{In}) - nE(\text{X}) \quad (1)$$

where $E(\text{In}_m\text{X}_n)$ is the total energy of the compound In_mX_n . $E(\text{In})$ and $E(\text{X})$ represent the total energy of In and X in their stable structures, respectively. The calculated results are summarized in Table 2.

4. Thermodynamic modeling

4.1 Unary phases

The Gibbs energy description of the pure element i ($i=\text{In}$, Sc or Y) in the phase ϕ has been given in the SGTE database [42] and the function is expressed by the following equation:

$$G_i^\phi - H_i^{\text{SER}} = a + bT + cT\ln T + dT^2 + eT^{-1} + fT^3 + gT^7 + hT^{-9} \quad (2)$$

where H_i^{SER} is the mole enthalpy of the element i at 25 °C and 1 bar in its standard element reference (SER) state, and T is the absolute temperature.

Table 2. Enthalpies of formation for the intermetallic compounds in the In–Y and In–Sc systems obtained by this work

System	Compound	ΔH_f (kJ/mol-atoms)	Method
In-Sc	InSc_3	-28.2	first-principles calculations
	InSc_2	-37.5	first-principles calculations
	InSc	-41.1	first-principles calculations
	In_2Sc	-36.3	first-principles calculations
	In_3Sc	-29.9	first-principles calculations
In-Y	InY_2	-39	first-principles calculations
	In_3Y_5	-41.9	first-principles calculations
	InY	-49.8	first-principles calculations
	In_5Y_3	-49.1	first-principles calculations
	In_3Y	-43.4	first-principles calculations

4.2 Solution phases

The liquid, (αSc), (βSc), (αY) and (βY) phases are modeled as completely disordered solutions. The Gibbs energy is described by Redlich-Kister polynomial [43]:

$$G^\phi - H^{\text{SER}} = x_{\text{In}}^0 G_{\text{In}}^\phi + x_i^0 G_i^\phi + RT(x_{\text{In}}\ln x_{\text{In}} + x_i\ln x_i) + x_{\text{In}}x_i \sum_{j=0}^n L_{\text{In},i}^{j,\phi} (x_{\text{In}} - x_i)^j \quad (3)$$

where $H^{\text{SER}} = x_{\text{In}}H_{\text{In}}^{\text{SER}} + x_iH_i^{\text{SER}}$, x_{In} and x_i are the mole fractions of In and component i ($i=\text{Sc}$, Y), respectively. $x_{\text{In}}^0 G_{\text{In}}^\phi + x_i^0 G_i^\phi$ suggests the mechanical mixing of the pure elements to the Gibbs energy. The middle term $RT(x_{\text{In}}\ln x_{\text{In}} + x_i\ln x_i)$ denotes the ideal entropy of mixing to the Gibbs energy and R is the gas constant. The last term $x_{\text{In}}x_i \sum_{j=0}^n L_{\text{In},i}^{j,\phi} (x_{\text{In}} - x_i)^j$ indicates the excess Gibbs energy. $L_{\text{In},i}^{j,\phi}$ is the j th interaction parameter between In and component i of the phase ϕ , and it is equal to $L_{\text{In},i}^{j,\phi} = a_j + b_jT$. The parameters, a_j and b_j , are to be optimized in the present work.



4.3 Compounds

InSc₃, InSc₂, In₄Sc₅, InSc, In₂Sc, In₃Sc, InY₂, InY, In₅Y₃, and In₃Y are modeled as stoichiometric compounds. The Gibbs energy of the compound In_mX_n (X=Sc or Y) is given by the following equation:

$$G^{\text{In}_m\text{X}_n} - mH_{\text{In}}^{\text{SER}} - nH_{\text{X}}^{\text{SER}} = m {}^0G_{\text{In}}^{\text{Tet-A6}} + n {}^0G_{\text{X}}^{\text{SER}} + a + bT \quad (4)$$

where *a* and *b* are the parameters to be optimized in the present work.

Considering the reported homogeneity ranges [10], In₃Y₅ are modeled with two-sublattice models, (In)_m(In,Y)_n, *m*, *n* represent the number of sites in each sublattice. The Gibbs energy of this compound can be described by the following equation:

$$G^{\text{In}_m\text{Y}_n} = {}^0G_{\text{In:Y}}^{\text{In}_m\text{Y}_n} y_{\text{Y}}^m + {}^0G_{\text{In:In}}^{\text{In}_m\text{Y}_n} y_{\text{In}}^m + nRT(y_{\text{In}}^m \ln y_{\text{In}}^m + y_{\text{Y}}^m \ln y_{\text{Y}}^m) + y_{\text{In}}^m y_{\text{Y}}^m {}^0L_{\text{In:In,Y}}^{\text{In}_m\text{Y}_n} \quad (5)$$

where the parameter y_i^j is the site fraction of the species *i* (*i* = In or Y) on the sublattice *j*. The superscript " " denote the second sublattices of the presented model.

${}^0G_{\text{In:Y}}^{\text{In}_m\text{Y}_n}$ and ${}^0G_{\text{In:In}}^{\text{In}_m\text{Y}_n}$ is the Gibbs energy of the ideal compound In₃Y₅ and In₃In₅, respectively. ${}^0G_{\text{In:Y}}^{\text{In}_m\text{Y}_n}$ and ${}^0G_{\text{In:In}}^{\text{In}_m\text{Y}_n}$ can be described as the equation (4).

5. Results and discussion

The first-principles calculated lattice parameters and formation enthalpies of the phases in the In–Sc and In–Y systems are shown in Table 1 and 2, respectively. Compared with the experimental lattice parameters, the first-principles results exhibit the deviation of 0.01%–4.47%, which is a good agreement.

Evaluation of the thermodynamic parameters was performed by the optimization program PARROT [44] of the Thermo-Calc software, which is based on minimizing the squared sum of differences between experimental values and computed ones. The step-by-step optimization procedure [45] was utilized in the present work. The reliable experimental data and the enthalpies of formation for the compounds via first-principles calculations were employed as input data. In the process of optimization, each piece of reliable input data was given a certain weight which was varied in different steps during the assessment.

Taking the In–Y system as an example, the optimization began with introducing InY₂ and In₃Y in the modeling one by one. In the first steps, the parameter *a* in Eq. (4) was set to be the Δ*H_f* calculated by the first-principles method because of its well-known good accuracy. Then, parameter *b* in Eq. (4)

for InY₂ and In₃Y was optimized using the invariant reactions and melting points. Subsequently, the other compounds, In₃Y₅, In₅Y₃, InY, and In₅Y₃ were introduced in the modeling one by one. The parameters *a* and *b* in Eq. (4) for these compounds were obtained as the same procedure. Meanwhile, the parameters for liquid, *a*₀, *a*₁, *a*₂, *b*₀, *b*₁, and *b*₂ in Eq. (3) were evaluated to fit for the experimental liquidus data. For (In) phase, the interaction parameters were fixed to be zero due to its negligible solubility ranges. For (αY) and (βY), which contain certain solubility ranges, its parameters were optimized using invariant reactions and experimental data. Finally, all the parameters were optimized simultaneously by taking into consideration all the phase equilibria and thermodynamic data. The procedure of optimization for the In–Sc system was analogous with that of the In–Y system. The optimized thermodynamic parameters are summarized in Table 4.

The calculated enthalpies of formation for the In–Sc and In–Y binary compounds are shown in the Fig. 1

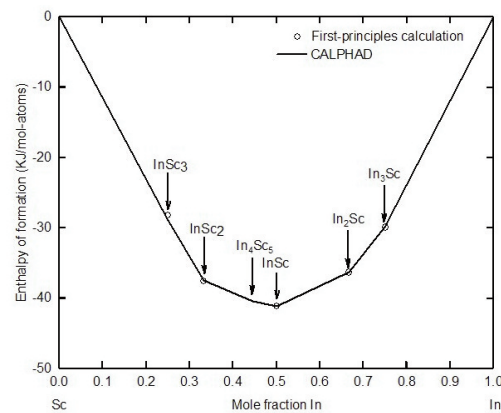


Figure 1. Enthalpies of formation for the In–Sc compounds at 25 °C compared with the first-principles results. The reference states are hcp Sc and tetragonal In

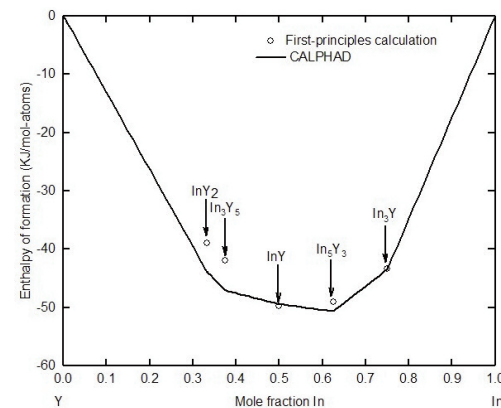


Figure 2. Enthalpies of formation for the In–Y compounds at 25 °C compared with the first-principles results. The reference states are hcp Y and tetragonal In

and Fig. 2, respectively, which are comparable with the first-principles results.

The calculated In–Sc and In–Y phase diagram compared with the experimental data [10, 18] are shown in the Fig. 3 and Fig. 4, respectively. The calculated invariant equilibria along with experimental data are listed in Table 3. Most of the experimental data can be well reproduced by the present calculation. In the In–Sc system, it is shown that the melting temperature of the InSc₂ is calculated to be 1397 °C, the eutectic reactions Liquid ↔ (βSc) + InSc₃ and Liquid ↔ In₃Sc + (In) are located at 1327 °C and 158 °C, respectively, the eutectoid reaction (βSc) ↔ (αSc) +

Table 3. Summary of invariant reactions in the In–Sc and In–Y systems obtained using the CALPHAD method in this work compared with the experimental data [10, 18]

System	Reaction	T(°C) ()	
		CALPHAD	Experiment
In–Sc	Liquid ↔ (βSc) + InSc ₃	1323(0.215)	1329(0.208) [18]
	(βSc) ↔ (αSc) + InSc ₃	1101(0.142)	1109(0.173) [18]
	Liquid + InSc ₂ ↔ InSc ₃	1338(0.255)	1348(0.220) [18]
	Liquid ↔ InSc ₂	1403(0.332)	1404(0.333) [18]
	Liquid + InSc ₂ ↔ In ₄ Sc ₅	1276(0.451)	1281(0.523) [18]
	Liquid + In ₄ Sc ₅ ↔ InSc	1123(0.596)	1140(0.609) [18]
	Liquid + InSc ↔ In ₂ Sc	967(0.7)	978(0.712) [18]
	Liquid + In ₂ Sc ↔ In ₃ Sc	932(0.766)	937(0.767) [18]
	Liquid ↔ In ₃ Sc + (In)	157(0.999)	148(0.999) [18]
In–Y	Liquid ↔ (βY) + InY ₂	1062(0.184)	1057(0.172) [10]
	(βY) ↔ (αY) + InY ₂	1031(0.118)	1022(0.119) [10]
	Liquid + In ₃ Y ₅ ↔ InY ₂	1322(0.334)	1331(0.329) [10]
	Liquid ↔ In ₃ Y ₅	1341(0.375)	1337(0.381) [10]
	Liquid + In ₃ Y ₅ ↔ InY	1214(0.501)	1219(0.500) [10]
	Liquid ↔ InY + In ₅ Y ₃	1131(0.580)	1088(0.557) [10]
	Liquid ↔ In ₅ Y ₃	1151(0.626)	1140(0.634) [10]
	Liquid ↔ In ₅ Y ₃ + In ₃ Y	1093(0.704)	1079(0.683) [10]
	Liquid ↔ In ₃ Y	1118(0.750)	1110(0.753) [10]
	Liquid ↔ In ₃ Y + (In)	157(0.999)	151(0.999) [10]

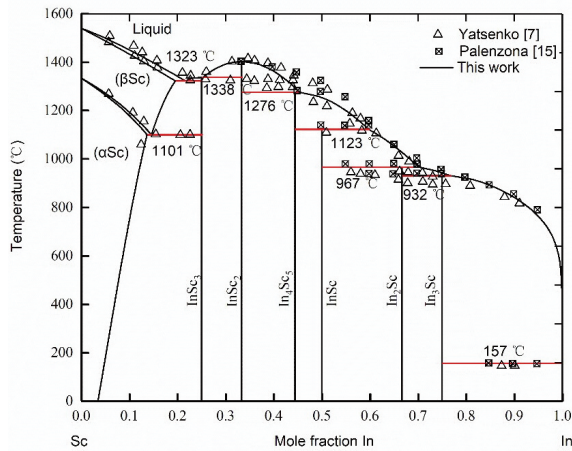


Figure 3. Calculated In–Sc phase diagram with the experimental data [10, 18]

InSc₃ is located at 1107 °C, the peritectic reactions Liquid + InSc₂ ↔ InSc₃, Liquid + InSc₂ ↔ In₄Sc₅, Liquid + In₄Sc₅ ↔ InSc, Liquid + InSc ↔ In₂Sc and Liquid + In₂Sc ↔ In₃Sc are located at 1347 °C, 1277 °C, 1127 °C, 967 °C and 937 °C, respectively. The deviation between the calculated and experimental invariant reaction points is less than 15 °C and 0.1 at.% In. In the In–Y systems, the melting temperature of the In₃Y₅, In₅Y₃, and In₃Y compounds are calculated to be 1337 °C, 1147 °C and 1107 °C, respectively. The eutectic points of four eutectic reactions Liquid ↔ (βY) + InY₂, Liquid ↔ InY + In₅Y₃, Liquid ↔ In₅Y₃ + In₃Y and Liquid ↔ In₃Y + (In) lie at 1057 °C, 1127 °C, 1087 °C and 158 °C, respectively. Two eutectoid reactions Liquid + In₃Y₅ ↔ InY₂, Liquid + In₃Y₅ ↔ InY are calculated to be 1317 °C and 1217 °C. The difference between the calculated and experimental data of the other invariant reaction is less than 15 °C and 0.1 at.% In, which is a good agreement. There is a large difference (39 °C) between the calculated (1127 °C) and reported (1088 °C) reaction point of the Liquid ↔ InY + In₅Y₃. The present calculation can be considered reasonable because the reported temperature is an assessed value of 9 DTA data points within the range from 1079 to 1136 °C.

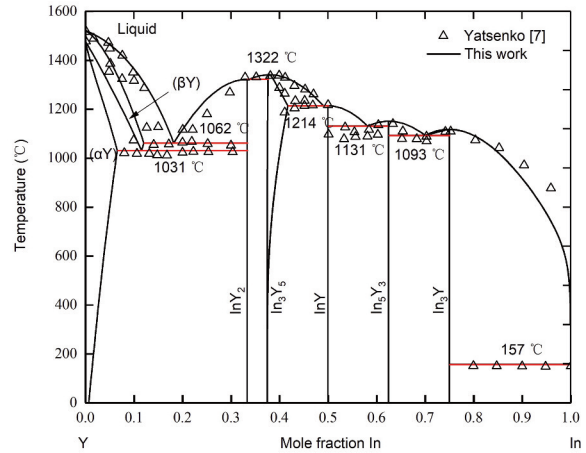


Figure 4. Calculated In–Y phase diagram with the experimental data [10]

6. Conclusions

(1) The experimental phase equilibria and thermodynamic data available for the In–Sc and In–Y systems were critically evaluated.

(2) The enthalpies of formation for InSc₃, InSc₂, In₄Sc₅, InSc, In₂Sc, In₃Sc, InY₂, In₃Y₅, InY, In₅Y₃, and In₃Y were obtained by means of first-principles calculations, which were also set as reliable input values used in the present thermodynamic modeling.

(3) A set of self-consistent thermodynamic parameters have been obtained to represent the phase



Table 4. Summary of the thermodynamic parameters in the In–Sc and In–Y systems*

System	Phase	Model	Parameters
In–Sc	Liquid	(In,Sc) ₁	${}^0L_{In,Sc}^{Liquid} = -96394.19$ ${}^1L_{In,Sc}^{Liquid} = 40221.46 - 9.80T$ ${}^2L_{In,Sc}^{Liquid} = 3200$
	(αSc)	(In,Sc) ₁ (Va) _{0.5}	${}^0L_{In,Sc:Va}^{HCP_{A3}} = -95743.42$ ${}^1L_{In,Sc:Va}^{HCP_{A3}} = 23197.63$ ${}^2L_{In,Sc:Va}^{HCP_{A3}} = 0$
	(βSc)	(In,Sc) ₁ (Va) ₃	${}^0L_{In,Sc:Va}^{BCC_{A2}} = -100806.23$ ${}^1L_{In,Sc:Va}^{BCC_{A2}} = 21202.68$ ${}^2L_{In,Sc:Va}^{BCC_{A2}} = 0$
	InSc ₃	(In) ₁ (Sc) ₃	${}^0G_{In:Sc}^{InSc_3} - {}^0G_{In}^{SER} - 3 {}^0G_{Sc}^{SER} = -115904.59$
	InSc ₂	(In) ₁ (Sc) ₂	${}^0G_{In:Sc}^{InSc_2} - {}^0G_{In}^{SER} - 2 {}^0G_{Sc}^{SER} = -112484.2 + 5.1171264T$
	In ₄ Sc ₅	(In) ₄ (Sc) ₅	${}^0G_{In:Sc}^{In_4Sc_5} - 4 {}^0G_{In}^{SER} - 5 {}^0G_{Sc}^{SER} = -363654.29 + 25.99T$
	InSc	(In) ₁ (Sc) ₁	${}^0G_{In:Sc}^{InSc} - {}^0G_{In}^{SER} - {}^0G_{Sc}^{SER} = -82200 + 8.69T$
	In ₂ Sc	(In) ₂ (Sc) ₁	${}^0G_{In:Sc}^{In_2Sc} - 2 {}^0G_{In}^{SER} - {}^0G_{Sc}^{SER} = -108889.46 + 18.98T$
	In ₃ Sc	(In) ₃ (Sc) ₁	${}^0G_{In:Sc}^{In_3Sc} - 3 {}^0G_{In}^{SER} - {}^0G_{Sc}^{SER} = -119572 + 19.04T$
In–Y	Liquid	(In,Y) ₁	${}^0L_{In,Y}^{Liquid} = -140405.32 - 8.95T$ ${}^1L_{In,Y}^{Liquid} = 8163.39 - 7.90T$ ${}^2L_{In,Y}^{Liquid} = 19055.86$
	(αY)	(In,Y) ₁ (Va) _{0.5}	${}^0L_{In,Y:Va}^{(HCP_{A3})} = -41830.67 - 37.39T$ ${}^1L_{In,Y:Va}^{HCP_{A3}} = 83504.65 - 40.39T$ ${}^2L_{In,Y:Va}^{HCP_{A3}} = 0$
	(βY)	(In,Y) ₁ (Va) ₃	${}^0L_{In,Y:Va}^{BCC_{A2}} = -127850.63 - 7.85T$ ${}^1L_{In,Y:Va}^{BCC_{A2}} = -6871.02$ ${}^2L_{In,Y:Va}^{BCC_{A2}} = 0$
	InY ₂	(In) ₁ (Y) ₂	${}^0G_{In:Y}^{InY_2} - {}^0G_{In}^{SER} - 2 {}^0G_Y^{SER} = -131712.82$
	In ₃ Y ₅	(In) ₃ (In,Y) ₅	${}^0G_{In:In}^{In_3Y_5} - 8 {}^0G_{In}^{SER} = 29300$
			${}^0G_{In:Y}^{In_3Y_5} - 3 {}^0G_{In}^{SER} - 5 {}^0G_Y^{SER} = -376332.85$ ${}^0L_{In:In,Y}^{In_3Y_5} = -254841.25 - 80.15T$
	InY	(In) ₁ (Y) ₁	${}^0G_{In:Y}^{InY} - {}^0G_{In}^{SER} - {}^0G_Y^{SER} = -98800.16 - 0.52T$
	In ₅ Y ₃	(In) ₅ (Y) ₃	${}^0G_{In:Y}^{In_5Y_3} - 5 {}^0G_{In}^{SER} - 3 {}^0G_Y^{SER} = -405314.16 + 19.19T$
	In ₃ Y	(In) ₃ (Y) ₁	${}^0G_{In:Y}^{In_3Y} - 3 {}^0G_{In}^{SER} - {}^0G_Y^{SER} = -173600 + 12T$

*Gibbs energies are in J·mol⁻¹. The Gibbs energies for the pure elements are from the SGTE compilation [42]

diagram of the In–Sc and In–Y systems by the CALPHAD method. A comprehensive comparison shows that the calculated phase diagram and thermodynamic properties are in good agreement with the experimental data and first-principles calculations.

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TERMODINAMIČKO MODELIRANJE In-Sc I In-Y SISTEMA PODRŽANO PRORAČUNIMA IZ PRVIH PRINCIPA

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Apstrakt

Na osnovu procene fazne ravnoteže i termodinamičkih podataka u literaturi, izvršeno je termodinamičko modeliranje In-Sc i In-Y sistema putem proračuna faznog dijagrama (CALPHAD) metode uz pomoć proračuna iz prvih principa. Faze rastvora, tj. tečne (In), (aSc), (βSc), (αY) i (βY) modelirane su modelom supstitucije regularnog rastvora. Deset intermetalnih komponenti, uključujući InSc₃, InSc₂, In₄Sc₃, InSc, In₂Sc, In₃Sc, InY₂, InY, In₃Y₃ i In₃Y, opisano je kao stehiometrijske faze, dok je In₃Y₃ modeliran modelom podrešetke u odnosu na raspon homogenosti. Entalpije formiranja intermetalnih komponenti pri 0 K izračunate su korišćenjem proračuna iz prvih principa, i upotrebljene kao input za termodinamičku optimizaciju. Dobijen je skup samoodrživih termodinamičkih parametara i za In-Sc, kao i za In-Y sistem, i proračunati fazni dijagrami se u velikoj meri slažu sa eksperimentalnim podacima.

Ključne reči: In-Sc; In-Y; Termodinamička optimizacija; Proračuni iz prvih principa; CALPHAD; Fazni dijagram

