Thermodynamic calculations of the Au-Sc and Fe-Sc systems

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Abstract

Thermodynamic optimization of the Au-Sc and Fe-Sc systems was carried out by means of the CALPHAD (CALculation of PHase Diagram) method on the basis of the available experimental data in literature. Redlich-Kister polynomials were used to describe the excess Gibbs energy of solution phases, and all the compounds are treated as stoichiometric ones. The Au-Sc system was described thermodynamically for the first time, and the Fe-Sc system was re-optimized by considering the new experimental data about enthalpies of mixing of the liquid phase. A set of self-consistent parameters was obtained for each of these two binary systems, respectively.

1 **Keywords:**

2 CALPHAD; Phase diagram; Au-Sc; Fe-Sc; Thermodynamic modeling

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4 **1. Introduction**

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6 Alloys with scandium addition have been considered to be a new generation of
7 high-performance alloy structural materials for aerospace, ships and weapons [1],
8 which is expected to have important advanced applications in many emerging
9 industry fields. The addition also does improvements on many other kind of alloys for
10 example to remove gases and other harmful impurities and reduce the occurrence of
11 cracks during solidification of alloys. With the addition of a small amount of
12 scandium, the tensile strength, elongation and hardness, as well as the corrosion and
13 heat resistance of aluminum alloys can be significantly improved [2]. In addition,
14 Fe-Sc alloys can be used as nanoglass material. Recently, Wang et al. [3] have
15 discussed the plasticity of the scandium-based nanoglass. Moreover, Scandium
16 addition into gold alloy can significantly strengthen alloy and raise the
17 recrystallization temperature [4]. The phase equilibria and thermodynamic properties
18 in the Au-Sc and Fe-Sc systems are of great importance for the designing of related
19 new materials. However, thermodynamic description about the Au-Sc system is
20 unavailable and the recently published thermodynamic description of the Fe-Sc
21 system [5] cannot be reproduced right using the provided parameters.

22 The present work is devoted to performing thermodynamic modeling of the Au-Sc

1 and Fe-Sc systems by considering the experimental data in literatures via CALPHAD
2 approach [6].

3 4 **2. Evaluation of the literature information**

5
6 The available literature data of phase diagram and thermodynamic properties on the
7 Au-Sc and Fe-Sc systems were critically reviewed in the present work and
8 summarized in Tables 1 and 2.

9 10 *2.1. The Au-Sc system*

11
12 The experimental data on phase equilibrium of the Au-Sc system are limited. The
13 Au-Sc phase diagram was originally reported by Palenzona et al. [7], in the
14 compositional range from 10 to 80 at. % Sc by means of differential thermal analysis
15 (DTA) and X-ray diffraction (XRD). Rider et al. [8] investigated the solubility of Sc
16 in (α Au) in the range from 0 to 10 at. % Sc by XRD and reported that the largest
17 solubility of Sc was up to 8.8 at. %, and the eutectic temperature reached 1040 °C.
18 Based on these data, Okamoto [9] reviewed the complete phase diagram. Generally,
19 there are three solution phases (α Au, α Sc and β Sc phases), and six intermetallic
20 compounds (Au_4Sc , Au_3Sc , Au_2Sc , AuSc , AuSc_2 and Au_2Sc_7) in the system as shown
21 in Table 1.

22 Kleppa and Topor [10] and Fitzner et al. [11] investigated the enthalpies of mixing

of the Au-Sc alloys at 1379 K and 1473 K by high-temperature reaction calorimetry (HTRC), respectively. Besides, Fitzner et al. [11] reported the standard enthalpy of formation of AuSc based on the observed heats of mixing and the average heat contents. Later, Wu et al. [12] calculated the formation enthalpies of disordered solid solutions and intermetallic compounds (Au_4Sc , Au_3Sc , Au_2Sc , AuSc and AuSc_2) at zero-temperature in the Au-Sc system with the modified analytical embedded atom method (EAM) [13, 14] and the first-principles calculations. All the available data for the Au-Sc system are summarized in Table 2.

2.2 The Fe-Sc system

The phase diagram was firstly experimentally investigated by Naumkin et al. [18]. Subsequently, Bodak et al. [19] reported the similar phase equilibria. Besides, Hellawell [20] measured the solubility of Sc in (αFe) and (δFe) in the range less than 1.5 at. % Sc. The phase diagram of Fe-Sc system was assessed by Okamoto [21]. There are five solution phases (αFe , γFe , δFe , αSc and βSc phases), and four intermetallic compounds ($\alpha\text{Fe}_2\text{Sc}$, $\beta\text{Fe}_2\text{Sc}$, $\lambda\text{Fe}_2\text{Sc}$, and $\text{Fe}_6\text{Sc}_{29}$) in the system, as listed in Table 1.

It should be mentioned that Bodak et al. [19] reported the formula of FeSc_7 for the compound with the composition of $\text{Fe}_6\text{Sc}_{29}$. However, in most recently studies, the composition of FeSc_7 was redefined as $\text{Fe}_6\text{Sc}_{29}$ [22], and the related peritectoid reaction temperature was 865 °C. So this phase is modeling as $\text{Fe}_6\text{Sc}_{29}$ in the present

1 work.

2 Partial and integral enthalpies of mixing of liquid Fe-Sc alloys were determined by
3 Sudavtsova et al. [23] and Esin et al. [24] at 1870 K up to 11 at. % Sc and 18 at. % Sc,
4 respectively. Most recently, the partial and integral mixing enthalpies of Fe-Sc melts
5 at 1873 K over the entire composition range were determined by Sudavtsova et al. [25]
6 by calorimetry. Enthalpies of formation for at the Fe_2Sc and $\text{Fe}_6\text{Sc}_{29}$ phases at 1473 K
7 have been experimentally determined using calorimetry by Selhaoui et al. [26] and
8 Savchenkova et al. [27]. Besides, Burylev [28] and Boer et al. [29] calculated
9 enthalpy formation of the Fe_2Sc phase using the Miedema and Hildebrand-Mott
10 models. All the experimental data for the Au-Sc system are summarized in Table 2.

11 The Fe-Sc system has been thermodynamically assessed by Liu et al. [5], as shown
12 in Fig. 1. Obviously, the latest experimental data investigated by Sudavtsova et al. [25]
13 was not considered in their work. There also exist some other calculation problems
14 using the published parameters. One is that the calculated temperature for the eutectic
15 reaction $\text{L} \leftrightarrow (\gamma\text{Fe}) + \beta\text{Fe}_2\text{Sc}$ was almost 30 °C lower, and the stable temperature range
16 of $\lambda\text{Fe}_2\text{Sc}$ was much larger than reported ones in literature [18, 19]. Another problem
17 is that the calculated liquidus curve around 50 at. % Sc was not fitted well and the
18 enthalpies of mixing in their calculation were much lower comparing to the literature
19 data [25]. All the problems mentioned before is due to one basic reason, the
20 parameters of liquid phase were inaccurate.

21 Recently, Sudavtsova et al. [25] plotted the liquidus curve for the Fe-Sc phase
22 diagram according to the model of ideal associated solutions (IAS) [30, 31] and their

thermodynamic parameters. Based on the effect of the IAS model, not only the trend of the liquidus curve, but also their eutectic reaction points and temperatures differed from the calculation carried out by Liu et al. [5].

It is essential to re-optimize this system, since the accurate thermodynamic description is very necessary for the establishment of aluminum alloy thermodynamic database and the development of advanced materials.

3. Thermodynamic modeling

3.1 Unary phases

The thermodynamic parameters of pure elements Au, Fe and Sc are taken from the SGTE-compilation by Dinsdale [34] described as follows:

$$G_i(T) - H_i^{SER} = A + B \times T + C \times T \times \ln T + D \times T^2 + E \times T^{-1} + F \times T^3 + I \times T^7 + J \times T^{-9} \quad (1)$$

Where, H_i^{SER} is the molar enthalpy of the pure element i at 298.15K and 1 bar in its standard element reference (SER) state, and T is the absolute temperature.

3.2 Solution phases

The liquid, (α Au), (α Fe), (γ Fe), (δ Fe), (α Sc) and (β Sc) phases are modeled as completely disordered solution phases, and their molar Gibbs energies are described

1 in the form of:

$$2 \quad G^\varphi - H^{SER} = x_{Tm} \times {}^0G_{Tm}^\varphi + x_{Sc} \times {}^0G_{Sc}^\varphi + R \times T \times (x_{Tm} \times \ln x_{Tm} + x_{Sc} \times$$

$$3 \quad \ln x_{Sc}) + x_{Tm} \times x_{Sc} \times L_{Tm,Sc}^\varphi \quad (2)$$

4 Where, x_{Tm} is the mole fraction of the element Tm (Tm=Au or Fe), and ${}^0G_{Tm}^\varphi$ is
 5 the Gibbs energy of element Tm under the state of φ . $L_{Tm,Sc}^\varphi$ stands for the
 6 interaction parameter in the form of the Redlich-Kister (R-K) polynomial [35]:

$$7 \quad L_{Tm,Sc}^\varphi = \sum_{i=0}^n L_{Tm,Sc}^{i,\varphi} \times (x_{Tm} - x_{Sc})^i \quad (3)$$

8 Where, $L_{Tm,Sc}^{i,\varphi} = a_i + b_i T$ is the i th interaction parameter of the solution phase φ
 9 in the Au–Sc and Fe–Sc systems, and a_i and b_i are the parameters that should be
 10 optimized in the present work.

11 The equation about the Fe–Sc system in Eq. (4) is the magnetic contribution to the
 12 Gibbs energy. For the liquid phase, ${}^{mag}G^\varphi$ is equal to zero, and for other solution
 13 phases, the magnetic contribution from pure Fe to the Gibbs energy is given by the
 14 Hillert–Jarl–Inden model [36]:

$$15 \quad G_m^{mag} = R \times T \times \ln(\beta^\varphi + 1) \times g(\tau^\varphi) \quad (4)$$

16 Where, β is the Bohr magnetic moment per mole atoms. As for the variable τ , there
 17 exists one expression, $\tau = T/T_c^*$, T_c^* is defined as the critical temperature for
 18 magnetic ordering (Curie or Neel temperature). The complete description of the
 19 function $g(\tau)$ is given in Ref. [36], as follows:

$$20 \quad g(\tau^\varphi) = 1 - \frac{\left[\frac{79\tau^{-1}}{140p} + \frac{474}{497} \left(\frac{1}{p-1} \right) \left(\frac{\tau^3}{6} + \frac{\tau^9}{135} + \frac{\tau^{15}}{600} \right) \right]}{D},$$

$$21 \quad \text{for } \tau \leq 1 \quad (5)$$

$$g(\tau^\varphi) = -\frac{(\tau^{-5}/10 + \tau^{-15}/315 + \tau^{-25}/1500)}{D},$$

for $\tau > 1$ (6)

$$D = \frac{518}{1125} + \frac{11692}{15975} \left(\frac{1}{p} - 1 \right)$$
(7)

Where, the parameter p depends on the structure, 0.40 for bcc structure and 0.28 for others.

6

3.3 Intermetallic phases

8

In these two systems, ten intermetallic compounds have been mentioned. Au₄Sc, Au₃Sc, Au₂Sc, AuSc, AuSc₂ and Au₂Sc₇ phases in the Au-Sc system, and αFe₂Sc, βFe₂Sc, λFe₂Sc, and Fe₆Sc₂₉ phases in the Fe-Sc system.

The Gibbs energy per mole atoms of $Tm_xSc_{(1-x)}$ compound is described as follow:

$${}^0G_m^{Tm_xSc_{1-x}} - x \times H_{Tm}^{SER} - (1-x) \times H_{Sc}^{SER} = a + b \times T + x \times {}^0G_{TM}^{SER} + (1-x) \times {}^0G_{Sc}^{Hcp}$$
(8)

In which, a and b are the parameters that needed to be optimized in this work.

17

4. Optimization procedure and results

19

The optimization of the thermodynamic parameters for these two systems was carried out by using the PARROT module of the Thermo-Calc software [37]. It was started with the liquid phase by using the experimental data of partial and integral

enthalpies of mixing. After that, the intermetallic compounds and other solution phases were taken into consideration one by one. All the intermetallic phases were treated as stoichiometric ones, and the experimentally measured enthalpies of formation for the intermetallic phases were used as good starting values for the parameters a in Eq. (8). Parameters a_i and b_i for the solution phases were introduced to describe the solubility ranges. At last all parameters for different phases were optimized simultaneously to achieve a globally self-consistent thermodynamic description. The finally obtained thermodynamic parameters are listed in Table 3.

4.1 The Au-Sc system

The calculated Au–Sc phase diagram using the present parameters is shown in Fig. 2, and compared with the experimental data taken from refs [7, 8]. Table 4 lists the invariant equilibria in the Au-Sc system. The experimental data of Sc-rich region is limited. Thus the solubility boundary of Au in solution phase (α Sc) and (β Sc) is taken to be zero in the optimization. In the range from 50 to 65 at. % Au, Palenzona et al. [7] observed a thermal effect at 1510 °C. Since this kind of behavior was not able to explain clearly, it is not taken into consideration in the present work.

Fig. 3 shows the calculated enthalpy of formation in the Au-Sc system at 298 K compared with the literature data [11, 12]. From the figure, we can see that the enthalpy of formation of the AuSc phase fits well to the experimental data, and the trends of other intermetallic phases are also reasonable to some extent.

Fig. 4 shows the calculated solid-liquid enthalpies of mixing of Au (l)+ Sc (s) at 1379 K and 1473 K compared with the experimental data [10, 11], and the calculated data is reasonable. As a result of dropping solid scandium into liquid gold in their experiments, the reference state of scandium in this work is taken as solid (α Sc). In the present work, temperature dependence of enthalpies is not taken into consideration due to the limited and dispersed experimental data below 1473 K.

4.2 The Fe-Sc system

The calculated Fe-Sc phase diagram based on the presently obtained thermodynamic parameters is shown in Fig. 5, and compared to the experimental data [18-20]. Table 4 shows the invariant equilibria in the Fe-Sc system.

In this work, the stable temperature range of λ Fe₂Sc locates between 1295 °C to 1525 °C, which fits well with the literature information [21]. In addition, the latest experimental data of enthalpy of mixing investigated by Sudavtsova et al. [25] are considered in the optimization of the liquid phase, which leads to the much better curvature of the liquidus, in comparison with the previous assessment [5]. According to the present calculations, the calculated temperatures for the eutectic reactions $L \leftrightarrow (\gamma\text{Fe}) + \beta\text{Fe}_2\text{Sc}$ and $L \leftrightarrow \alpha\text{Fe}_2\text{Sc} + (\alpha\text{Sc})$ are 1280 °C and 975 °C, which are different from the Fe-Sc phase diagram plotted according to the IAS model [25].

Fig. 6 presents the calculated enthalpies of formation at 298 K in the Fe-Sc system compared with the literature data [26-29]. Several different literature data about the

enthalpy of formation of Fe_2Sc located in a really large energy region. The data from the work of Selhaoui et al. [26] and Boer et al. [29] were more exothermic than those reported in others [27, 28]. The present calculation can reproduce the data from Selhaoui et al. [26] reasonably.

Fig. 7 shows the calculated integral and partial molar enthalpies of mixing for liquid at 1873 K compared with the experimental data [23-25]. The experimental data reported by Sudavtsova et al. [25] for partial enthalpies of mixing distributes pretty discrete, while the calculated result passes through the central region of these dots, and goes pretty well.

5. Summary

All the literature phase diagram data and thermodynamic data of the Au-Sc and Fe-Sc binary systems on the literature were critically evaluated in this work. A set of thermodynamic parameters for each of the Au-Sc and Fe-Sc systems was obtained based on the CALPHAD method, respectively. The comparison between calculations and experiments shows that the calculations can reproduce the experimental data reasonably.

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- 9

1 **Table 1**

2 Phases, structures and models of Au-Sc and Fe-Sc alloys.

Phase	Structure type	Lattice constants(Å)			Ref.
		a	b	c	
Au-Sc					
(αAu)	Cu	-	-	-	-
Au ₄ Sc	MoNi ₄	6.546	-	4.037	[7]
	tI10-I4/m	5.549	-	4.039	[9][15]
Au ₃ Sc	TiCu ₃	5.800	4.823	5.003	[7]
	oP8-Pmmn				-
Au ₂ Sc	MoSi ₂	3.510	-	8.728	[7]
	tI6-I4/mmm	3.509	-	8.730	[9][15]
AuSc	CsCl	3.369	-	-	[7]
	cP2-Pm3m	3.370	-	-	[9][15][16]
AuSc ₂	PbCl ₂	6.470	4.667	8.358	[7]
	oP12-Pnma	-	-	-	[17]
Au ₂ Sc ₇	PbCl ₂	14.360	14.360	14.360	[7]
	oI142-Immm	-	-	-	-
(αSc)	Mg	-	-	-	-
(βSc)	W	-	-	-	-
Fe-Sc					
(αFe)	W	-	-	-	-
(γFe)	Cu	-	-	-	-
(δFe)	W	-	-	-	-
βFe ₂ Sc	MgNi ₂	4.974	4.974	16.29	[32]
αFe ₂ Sc	MgZn ₂	4.948	4.948	8.077	[33]
λFe ₂ Sc	Cu ₂ Mg	7.039	7.039	7.039	[32]
Fe ₆ Sc ₂₉	Fe ₆ Sc ₂₉	14.361	14.361	14.361	[32]
(αSc)	Mg	-	-	-	-
(βSc)	W	-	-	-	-

3

4 **Table 2**

5 Summary of the literature data for the Au-Sc and Fe-Sc system.

Type of data	Reference	Method	Quoted mode
Au-Sc			
Liquidus			
10-80 at.% Sc	[7]	DTA	■
Solubility			
Sc in (α Au)	[8]	XRD	■

Homogeneity of different compounds			
Au ₄ Sc	[7]	XRD and MA	■
	[9][15]	XRD	□
Au ₃ Sc	[7]	XRD and MA	■
Au ₂ Sc	[7]	XRD and MA	■
	[9] [15]	XRD	□
AuSc	[7]	XRD and MA	■
	[9] [15]	XRD	□
AuSc ₂	[7]	XRD and MA	■
Au ₂ Sc ₇	[7]	XRD and MA	■
Eutectic temperature	[7]	DTA	■
Peritectic temperature	[7]	DTA	■
Enthalpies of formation	[11]	High tem. calorimetry	■
	[12]	EAM	□
	[12]	VASP	□
	[11]	Miedema	+
Enthalpy of mixing of liquid	[10] [11]	High tem. calorimetry	■
	[11]	Miedema	+
<hr/> Fe-Sc <hr/>			
Liquidus			
0-100 at.% Sc	[18]	DTA	■
0-80 at. % Sc	[19]	DTA	■
Solubility			
Sc in (α Fe) and (δ Fe)	[20]	XRD, MA and DTA	■
Homogeneity of different compounds			
α Fe ₂ Sc	[33]	XRD	■
β Fe ₂ Sc	[32]	XRD	■
λ Fe ₂ Sc	[32]	XRD	■
Fe ₆ Sc ₂₉	[32]	XRD	■
Eutectic temperature	[18]	DTA	■
	[19]	DTA	■
Peritectic temperature	[18]	DTA	■
	[19]	DTA	■
Enthalpies of formation	[26]	High tem. calorimetry	■
	[27]	High tem. calorimetry	+
	[28]	Miedema	+
	[29]	Hildebrand-Mott models	+
Partial and integral enthalpy of mixing	[23]	High tem. calorimetry	■
	[24]	High tem. calorimetry	□
	[25]	High tem. calorimetry	■

^a DTA: differential thermal analysis; MA: metallographic analysis; XRD: X-ray diffraction.

^b Indicates whether the data are used or not used in the optimization procedure: ■, used; □, not used but considered as reliable data for checking the modeling; +, not used.

6

Table 3

Thermodynamic parameters in the Au–Sc and Fe–Sc system.

Phase	Parameters
Au-Sc	
Liquid	${}^0L_{Au,Sc}^{Liquid} = -229326.82 + 8.12 \times T$ ${}^1L_{Au,Sc}^{Liquid} = -37303.77 - 14.29 \times T$ ${}^2L_{Au,Sc}^{Liquid} = 3441.85 + 2.39 \times T$
Fcc	${}^0L_{Au,Sc}^{Fcc} = -175520.06 - 22.02 \times T$ ${}^1L_{Au,Sc}^{Fcc} = -65519.78$
Au ₄ Sc	${}^0G_{Au,Sc}^{Au_4Sc} = 0.80 \times {}^0G_{Au}^{Bcc} + 0.20 \times {}^0G_{Sc}^{Hcp} - 54000 + 4.65 \times T$
Au ₃ Sc	${}^0G_{Au,Sc}^{Au_3Sc} = 0.75 \times {}^0G_{Au}^{Bcc} + 0.25 \times {}^0G_{Sc}^{Hcp} - 60000 + 3.25 \times T$
Au ₂ Sc	${}^0G_{Au,Sc}^{Au_2Sc} = 0.67 \times {}^0G_{Au}^{Bcc} + 0.33 \times {}^0G_{Sc}^{Hcp} - 66986.43 + 0.54 \times T$
AuSc	${}^0G_{Au,Sc}^{AuSc} = 0.50 \times {}^0G_{Au}^{Bcc} + 0.50 \times {}^0G_{Sc}^{Hcp} - 76100 + 3.70 \times T$
AuSc ₂	${}^0G_{Au,Sc}^{AuSc_2} = 0.33 \times {}^0G_{Au}^{Bcc} + 0.67 \times {}^0G_{Sc}^{Hcp} - 63000 + 7.72 \times T$
Au ₂ Sc ₇	${}^0G_{Au,Sc}^{Au_2Sc_7} = 0.22 \times {}^0G_{Au}^{Bcc} + 0.78 \times {}^0G_{Sc}^{Hcp} - 53000 + 12.50 \times T$
Fe-Sc	
Liquid	${}^0L_{Fe,Sc}^{Liquid} = -49300 - 14.2 \times T$ ${}^1L_{Fe,Sc}^{Liquid} = -7000 - 5.3 \times T$

$$\begin{aligned}
& {}^2L_{Fe,Sc}^{Liquid} = 8000 \\
\text{Fcc} \quad & {}^0L_{Fe,Sc}^{Fcc} = -57180 + 4.7 \times T \\
\text{Bcc} \quad & {}^0L_{Fe,Sc}^{Bcc} = -52280 + 13.8 \times T \\
& {}^1L_{Fe,Sc}^{Bcc} = -16220 \\
\text{Hcp} \quad & {}^0L_{Fe,Sc}^{Hcp} = 3700 \\
\alpha\text{Fe}_2\text{Sc} \quad & {}^0G_{Fe,Sc}^{\alpha\text{Fe}_2\text{Sc}} = 0.67 \times {}^0G_{Fe}^{Bcc} + 0.33 \times {}^0G_{Sc}^{Hcp} - 41266 + 7.3 \times T \\
& T_C^{\alpha\text{Fe}_2\text{Sc}} = 542 \\
& \beta^{\alpha\text{Fe}_2\text{Sc}} = 1.37 \\
\beta\text{Fe}_2\text{Sc} \quad & {}^0G_{Fe,Sc}^{\beta\text{Fe}_2\text{Sc}} = 0.67 \times {}^0G_{Fe}^{Bcc} + 0.33 \times {}^0G_{Sc}^{Hcp} - 41070 + 7.2 \times T \\
\lambda\text{Fe}_2\text{Sc} \quad & {}^0G_{Fe,Sc}^{\lambda\text{Fe}_2\text{Sc}} = 0.64 \times {}^0G_{Fe}^{Bcc} + 0.36 \times {}^0G_{Sc}^{Hcp} - 33195 + 2.6 \times T \\
\text{Fe}_6\text{Sc}_{29} \quad & {}^0G_{Fe,Sc}^{\text{Fe}_6\text{Sc}_{29}} = 0.17 \times {}^0G_{Fe}^{Bcc} + 0.83 \times {}^0G_{Sc}^{Hcp} - 12410 + 3.5 \times T
\end{aligned}$$

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2 **Table 4**

3 Summary of the invariant equilibria in the Au-Sc and Fe-Sc system.

Reaction	T(K)		Type	Phase	Composition, at. %Sc	
	Exp.[7] [21]	Calc.			Exp.[7][8][21]	Calc.
Au-Sc						
L↔ Au ₄ Sc+ (αAu)	1313	1306	eutectoid	L	8.8~14	10.1
				Au ₄ Sc	20	20
				(αAu)	0~8.8	9.4
L+ Au ₃ Sc↔ Au ₄ Sc	1498	1498	peritectic	L	17.2	17.9
				Au ₃ Sc	25	25
				Au ₄ Sc	20	20
L+ Au ₂ Sc↔ Au ₃ Sc	1578	1580	peritectic	L	22.8	21.8
				Au ₂ Sc	33.3	33.3
				Au ₃ Sc	25	25
L↔ Au ₂ Sc	1888	1885	congruent	L	33.3	33.3
				Au ₂ Sc	33.3	33.3
L↔ AuSc+ Au ₂ Sc	1798	1804	eutectoid	L	39.5	39.7
				AuSc	50	50
				Au ₂ Sc	33.3	33.3
L↔ AuSc	1973	1973	congruent	L	50	50
				AuSc	50	50

L+ AuSc $\leftrightarrow$ AuSc ₂	1548	1546	peritectic	L	70	69.1
				AuSc	50	50
				AuSc ₂	66.7	66.7
L+AuSc ₂ $\leftrightarrow$ Au ₂ Sc ₇	1408	1407	peritectic	L	81.2	80.1
				AuSc ₂	66.7	66.7
				Au ₂ Sc ₇	77.8	77.8
L $\leftrightarrow$ Au ₂ Sc ₇ + (α Sc)	1388	1389	eutectoid	L	82.2	84.5
				Au ₂ Sc ₇	77.8	77.8
				(α Sc)	98~100	100
Fe-Sc						
L $\leftrightarrow$ (δ Fe)	1811	1811	melting	L	100	100
				(δ Fe)	100	100
(δ Fe) $\leftrightarrow$ (γ Fe)	1668	1668	allotropic	(δ Fe)	100	100
				(γ Fe)	100	100
(δ Fe) $\leftrightarrow$ (γ Fe)+L	1653	1653	peritectic	(δ Fe)	-	-
				(γ Fe)	-	1.07
				L	-	6.73
(γ Fe) $\leftrightarrow$ (α Fe)	1185	1185	allotropic	(γ Fe)	100	100
				(α Fe)	100	100
(γ Fe)+ α Fe ₂ Sc $\leftrightarrow$ (α Fe)	1208	1208	peritectoid	(γ Fe)	-	0.59
				α Fe ₂ Sc	33.3	33.3
				(α Fe)	-	0.75
L $\leftrightarrow$ (γ Fe)+ β Fe ₂ Sc	1553	1553	eutectic	L	11.5	10.4
				(γ Fe)	-	2.58
				β Fe ₂ Sc	33.3	33.3
L $\leftrightarrow$ β Fe ₂ Sc	1838	1838	congruent	L	33.3	33.3
				β Fe ₂ Sc	33.3	33.3
β Fe ₂ Sc $\leftrightarrow$ α Fe ₂ Sc	1473	1473	poly- morphic	β Fe ₂ Sc	33.3	33.3
				α Fe ₂ Sc	33.3	33.3
L+ β Fe ₂ Sc $\leftrightarrow$ λ Fe ₂ Sc	1798	1798	peritectic	L	-	42.0
				β Fe ₂ Sc	33.3	33.3
				λ Fe ₂ Sc	35.7	36.0
λ Fe ₂ Sc $\leftrightarrow$ β Fe ₂ Sc+ L	1568	1568	peritectic	λ Fe ₂ Sc	35.7	36.0
				β Fe ₂ Sc	33.3	33.3
				L	39.0	57.9
L $\leftrightarrow$ α Fe ₂ Sc+ (α Sc)	1248	1248	eutectic	L	74.0	73.6
				α Fe ₂ Sc	33.3	33.3
				(α Sc)	-	99.5
α Fe ₂ Sc+(α Sc) $\leftrightarrow$ Fe ₆ Sc ₂₉	1138	1139	peritectoid	α Fe ₂ Sc	33.3	33.3

				(α Sc)	-	99.7
				Fe ₆ Sc ₂₉	87.5	83.0
L $\leftrightarrow$ (β Sc)	1814	1814	melting	L	0	0
				(β Sc)	0	0
(β Sc) $\leftrightarrow$ (α Sc)	1610	1610	poly- morphic	(β Sc)	0	0
				(α Sc)	0	0
(β Sc) $\leftrightarrow$ L+ (α Sc)	1544	1544	peritectic	(β Sc)	-	98.6
				L	-	85.3
				(α Sc)	-	99.7

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Figures Captions

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Fig. 1. The phase diagram of the Fe–Sc system calculated using the parameters of Liu et al. [5] comparing with the experimental results [18-20].

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Fig. 2. The calculated phase diagram of the Au–Sc system compared with the experimental data [7, 8].

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Fig. 3. Calculated Enthalpy of formation in the Au-Sc system with experiment data from Fitzner et al. [11] and Calculation from Wu et al. [12] by using EAM and the first-principles calculations.

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Fig. 4. Calculated solid-liquid enthalpies of mixing of Au(l)+ Sc(s) at 1379 K and 1473 K with experiment data [10, 11].

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Fig. 5. The calculated phase diagram of the Fe–Sc system compared with the

1 experimental data [18-20].

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3 **Fig. 6.** Calculated enthalpies of formation in the Fe-Sc system with experiment data
4 evaluated in Selhaoui et al. [26], Savchenkova et al. [27] by calorimetry and
5 Calculated in Burylev et al. [28], Boer et al. [29] using the Miedema and
6 Hildebrand-Mott models .

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8 **Fig. 7.** Calculated mixing integral and partial enthalpies of liquid phase at 1873 K, (a)
9 with experiment data from Esin et al. [24] and Sudavtsova et al. [25], (b) with
10 experiment data determined by Sudavtsova et al. [23, 25] at 1870 K up to 11 at% Sc
11 and by Esin et al. [24] up to 18 at% Sc.

1 **Table 1**
2 Phases, structures and models of Au-Sc and Fe-Sc alloys.

Phase	Structure type	Lattice constants(Å)			Ref.
		a	b	c	
Au-Sc					
(αAu)	Cu	-	-	-	-
Au ₄ Sc	MoNi ₄	6.546	-	4.037	[7]
	tI10-I4/m	5.549	-	4.039	[9][15]
Au ₃ Sc	TiCu ₃	5.800	4.823	5.003	[7]
	oP8-Pmmn				-
Au ₂ Sc	MoSi ₂	3.510	-	8.728	[7]
	tI6-I4/mmm	3.509	-	8.730	[9][15]
AuSc	CsCl	3.369	-	-	[7]
	cP2-Pm3m	3.370	-	-	[9][15][16]
AuSc ₂	PbCl ₂	6.470	4.667	8.358	[7]
	oP12-Pnma	-	-	-	[17]
Au ₂ Sc ₇	PbCl ₂	14.360	14.360	14.360	[7]
	oI142-Immm	-	-	-	-
(αSc)	Mg	-	-	-	-
(βSc)	W	-	-	-	-
Fe-Sc					
(αFe)	W	-	-	-	-
(γFe)	Cu	-	-	-	-
(δFe)	W	-	-	-	-
βFe ₂ Sc	MgNi ₂	4.974	4.974	16.29	[32]
αFe ₂ Sc	MgZn ₂	4.948	4.948	8.077	[33]
λFe ₂ Sc	Cu ₂ Mg	7.039	7.039	7.039	[32]
Fe ₆ Sc ₂₉	Fe ₆ Sc ₂₉	14.361	14.361	14.361	[32]
(αSc)	Mg	-	-	-	-
(βSc)	W	-	-	-	-

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1 **Table 2**

2 Summary of the literature data for the Au-Sc and Fe-Sc system.

Type of data	Reference	Method	Quoted mode
Au-Sc			
Liquidus			
10-80 at.% Sc	[7]	DTA	■
Solubility			
Sc in (α Au)	[8]	XRD	■
Homogeneity of different compounds			
Au ₄ Sc	[7]	XRD and MA	■
	[9][15]	XRD	□
Au ₃ Sc	[7]	XRD and MA	■
Au ₂ Sc	[7]	XRD and MA	■
	[9] [15]	XRD	□
AuSc	[7]	XRD and MA	■
	[9] [15]	XRD	□
AuSc ₂	[7]	XRD and MA	■
Au ₂ Sc ₇	[7]	XRD and MA	■
Eutectic temperature	[7]	DTA	■
Peritectic temperature	[7]	DTA	■
Enthalpies of formation	[11]	High tem. calorimetry	■
	[12]	EAM	□
	[12]	VASP	□
	[11]	Miedema	+
Enthalpy of mixing of liquid	[10] [11]	High tem. calorimetry	■
	[11]	Miedema	+
Fe-Sc			
Liquidus			
0-100 at.% Sc	[18]	DTA	■
0-80 at. % Sc	[19]	DTA	■
Solubility			
Sc in (α Fe) and (δ Fe)	[20]	XRD, MA and DTA	■
Homogeneity of different compounds			
α Fe ₂ Sc	[33]	XRD	■
β Fe ₂ Sc	[32]	XRD	■
λ Fe ₂ Sc	[32]	XRD	■
Fe ₆ Sc ₂₉	[32]	XRD	■
Eutectic temperature	[18]	DTA	■
	[19]	DTA	■

Peritectic temperature	[18]	DTA	■
	[19]	DTA	■
Enthalpies of formation	[26]	High tem. calorimetry	■
	[27]	High tem. calorimetry	+
	[28]	Miedema	+
	[29]	Hildebrand-Mott models	+
Partial and integral enthalpy of mixing	[23]	High tem. calorimetry	■
	[24]	High tem. calorimetry	□
	[25]	High tem. calorimetry	■

1 ^a DTA: differential thermal analysis; MA: metallographic analysis; XRD: X-ray
2 diffraction.

3 ^b Indicates whether the data are used or not used in the optimization procedure: ■,
4 used; □, not used but considered as reliable data for checking the modeling; +, not
5 used.

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1 **Table 3**

2 Thermodynamic parameters in the Au–Sc and Fe–Sc system.

Phase	Parameters
Au-Sc	
Liquid	${}^0L_{Au,Sc}^{Liquid} = -229326.82 + 8.12 \times T$
	${}^1L_{Au,Sc}^{Liquid} = -37303.77 - 14.29 \times T$
	${}^2L_{Au,Sc}^{Liquid} = 3441.85 + 2.39 \times T$
Fcc	${}^0L_{Au,Sc}^{Fcc} = -175520.06 - 22.02 \times T$
	${}^1L_{Au,Sc}^{Fcc} = -65519.78$
Au ₄ Sc	${}^0G_{Au,Sc}^{Au_4Sc} = 0.80 \times {}^0G_{Au}^{Bcc} + 0.20 \times {}^0G_{Sc}^{Hcp} - 54000 + 4.65 \times T$
Au ₃ Sc	${}^0G_{Au,Sc}^{Au_3Sc} = 0.75 \times {}^0G_{Au}^{Bcc} + 0.25 \times {}^0G_{Sc}^{Hcp} - 60000 + 3.25 \times T$
Au ₂ Sc	${}^0G_{Au,Sc}^{Au_2Sc} = 0.67 \times {}^0G_{Au}^{Bcc} + 0.33 \times {}^0G_{Sc}^{Hcp} - 66986.43 + 0.54 \times T$
AuSc	${}^0G_{Au,Sc}^{AuSc} = 0.50 \times {}^0G_{Au}^{Bcc} + 0.50 \times {}^0G_{Sc}^{Hcp} - 76100 + 3.70 \times T$
AuSc ₂	${}^0G_{Au,Sc}^{AuSc_2} = 0.33 \times {}^0G_{Au}^{Bcc} + 0.67 \times {}^0G_{Sc}^{Hcp} - 63000 + 7.72 \times T$
Au ₂ Sc ₇	${}^0G_{Au,Sc}^{Au_2Sc_7} = 0.22 \times {}^0G_{Au}^{Bcc} + 0.78 \times {}^0G_{Sc}^{Hcp} - 53000 + 12.50 \times T$
Fe-Sc	
Liquid	${}^0L_{Fe,Sc}^{Liquid} = -49300 - 14.2 \times T$
	${}^1L_{Fe,Sc}^{Liquid} = -7000 - 5.3 \times T$
	${}^2L_{Fe,Sc}^{Liquid} = 8000$
Fcc	${}^0L_{Fe,Sc}^{Fcc} = -57180 + 4.7 \times T$
Bcc	${}^0L_{Fe,Sc}^{Bcc} = -52280 + 13.8 \times T$
	${}^1L_{Fe,Sc}^{Bcc} = -16220$
Hcp	${}^0L_{Fe,Sc}^{Hcp} = 3700$
α Fe ₂ Sc	${}^0G_{Fe,Sc}^{\alpha Fe_2Sc} = 0.67 \times {}^0G_{Fe}^{Bcc} + 0.33 \times {}^0G_{Sc}^{Hcp} - 41266 + 7.3 \times T$
	$T_C^{\alpha Fe_2Sc} = 542$

$$\beta^{Fe_2Sc} = 1.37$$

$$\beta Fe_2Sc \quad {}^0G_{Fe,Sc}^{Fe_2Sc} = 0.67 \times {}^0G_{Fe}^{Bcc} + 0.33 \times {}^0G_{Sc}^{Hcp} - 41070 + 7.2 \times T$$

$$\lambda Fe_2Sc \quad {}^0G_{Fe,Sc}^{Fe_2Sc} = 0.64 \times {}^0G_{Fe}^{Bcc} + 0.36 \times {}^0G_{Sc}^{Hcp} - 33195 + 2.6 \times T$$

$$Fe_6Sc_{29} \quad {}^0G_{Fe,Sc}^{Fe_6Sc_{29}} = 0.17 \times {}^0G_{Fe}^{Bcc} + 0.83 \times {}^0G_{Sc}^{Hcp} - 12410 + 3.5 \times T$$

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1 **Table 4**

2 Summary of the invariant equilibria in the Au-Sc and Fe-Sc system.

Reaction	T(K)		Type	Phase	Composition, at. %Sc	
	Exp.[7] [21]	Calc.			Exp.[7][8][21]	Calc.
Au-Sc						
L↔ Au ₄ Sc+ (αAu)	1313	1306	eutectoid	L	8.8~14	10.1
				Au ₄ Sc	20	20
				(αAu)	0~8.8	9.4
L+ Au ₃ Sc↔ Au ₄ Sc	1498	1498	peritectic	L	17.2	17.9
				Au ₃ Sc	25	25
				Au ₄ Sc	20	20
L+ Au ₂ Sc↔ Au ₃ Sc	1578	1580	peritectic	L	22.8	21.8
				Au ₂ Sc	33.3	33.3
				Au ₃ Sc	25	25
L↔ Au ₂ Sc	1888	1885	congruent	L	33.3	33.3
				Au ₂ Sc	33.3	33.3
L↔ AuSc+ Au ₂ Sc	1798	1804	eutectoid	L	39.5	39.7
				AuSc	50	50
				Au ₂ Sc	33.3	33.3
L↔ AuSc	1973	1973	congruent	L	50	50
				AuSc	50	50
L+ AuSc↔ AuSc ₂	1548	1546	peritectic	L	70	69.1
				AuSc	50	50
				AuSc ₂	66.7	66.7
L+AuSc ₂ ↔Au ₂ Sc ₇	1408	1407	peritectic	L	81.2	80.1
				AuSc ₂	66.7	66.7
				Au ₂ Sc ₇	77.8	77.8
L↔Au ₂ Sc ₇ + (αSc)	1388	1389	eutectoid	L	82.2	84.5
				Au ₂ Sc ₇	77.8	77.8
				(αSc)	98~100	100
Fe-Sc						
L↔ (δFe)	1811	1811	melting	L	100	100
				(δFe)	100	100
(δFe)↔ (γFe)	1668	1668	allotropic	(δFe)	100	100
				(γFe)	100	100
(δFe)↔ (γFe)+L	1653	1653	peritectic	(δFe)	-	-
				(γFe)	-	1.07
				L	-	6.73
(γFe)↔ (αFe)	1185	1185	allotropic	(γFe)	100	100

				(α Fe)	100	100
(γ Fe)+ α Fe ₂ Sc $\leftrightarrow$ (α Fe)	1208	1208	peritectoid	(γ Fe)	-	0.59
				α Fe ₂ Sc	33.3	33.3
				(α Fe)	-	0.75
L $\leftrightarrow$ (γ Fe)+ β Fe ₂ Sc	1553	1553	eutectic	L	11.5	10.4
				(γ Fe)	-	2.58
				β Fe ₂ Sc	33.3	33.3
L $\leftrightarrow$ β Fe ₂ Sc	1838	1838	congruent	L	33.3	33.3
				β Fe ₂ Sc	33.3	33.3
β Fe ₂ Sc $\leftrightarrow$ α Fe ₂ Sc	1473	1473	poly- morphic	β Fe ₂ Sc	33.3	33.3
				α Fe ₂ Sc	33.3	33.3
L+ β Fe ₂ Sc $\leftrightarrow$ λ Fe ₂ Sc	1798	1798	peritectic	L	-	42.0
				β Fe ₂ Sc	33.3	33.3
				λ Fe ₂ Sc	35.7	36.0
λ Fe ₂ Sc $\leftrightarrow$ β Fe ₂ Sc+ L	1568	1568	peritectic	λ Fe ₂ Sc	35.7	36.0
				β Fe ₂ Sc	33.3	33.3
				L	39.0	57.9
L $\leftrightarrow$ α Fe ₂ Sc+ (α Sc)	1248	1248	eutectic	L	74.0	73.6
				α Fe ₂ Sc	33.3	33.3
				(α Sc)	-	99.5
α Fe ₂ Sc+ (α Sc) $\leftrightarrow$ Fe ₆ Sc ₂₉	1138	1139	peritectoid	α Fe ₂ Sc	33.3	33.3
				(α Sc)	-	99.7
				Fe ₆ Sc ₂₉	87.5	83.0
L $\leftrightarrow$ (β Sc)	1814	1814	melting	L	0	0
				(β Sc)	0	0
(β Sc) $\leftrightarrow$ (α Sc)	1610	1610	poly- morphic	(β Sc)	0	0
				(α Sc)	0	0
(β Sc) $\leftrightarrow$ L+ (α Sc)	1544	1544	peritectic	(β Sc)	-	98.6
				L	-	85.3
				(α Sc)	-	99.7

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Figures Captions

Fig. 1. The phase diagram of the Fe–Sc system calculated using the parameters of Liu et al. [5] comparing with the experimental results [18-20].

Fig. 2. The calculated phase diagram of the Au–Sc system compared with the experimental data [7, 8].

Fig. 3. Calculated Enthalpy of formation in the Au-Sc system with experiment data from Fitzner et al. [11] and Calculation from Wu et al. [12] by using EAM and the first-principles calculations.

Fig. 4. Calculated solid-liquid enthalpies of mixing of Au(l)+ Sc(s) at 1379 K and 1473 K with experiment data [10, 11].

Fig. 5. The calculated phase diagram of the Fe–Sc system compared with the experimental data [18-20].

Fig. 6. Calculated enthalpies of formation in the Fe-Sc system with experiment data evaluated in Selhaoui et al. [26], Savchenkova et al. [27] by calorimetry and Calculated in Burylev et al. [28], Boer et al. [29] using the Miedema and Hildebrand-Mott models .

1 **Fig. 7.** Calculated mixing integral and partial enthalpies of liquid phase at 1873 K, (a)
2 with experiment data from Esin et al. [24] and Sudavtsova et al. [25], (b) with
3 experiment data determined by Sudavtsova et al. [23, 25] at 1870 K up to 11 at% Sc
4 and by Esin et al. [24] up to 18 at% Sc.
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Figure 1

Figure 2

Figure 3

Figure 4

Figure 5

Figure 6

Figure 7a

Figure 7b