Journal of Mining and Metallurgy 44 B (2008) 49 - 61

Journal of
Mining and
Metallurgy

THERMODYNAMIC CALCULATIONS IN ALLOYS Ti-Al, Ti-Fe, Al-Fe AND Ti-Al-Fe

A. Kostov* , B. Friedrich and D. Živković*****

*Mining and Metallurgy Institute Bor, Zeleni bulevar 35, 19210 Bor, Serbia,
**RWTH Aachen, IME Metallurgische Prozesstechnik und
Metallrecycling Intzestrasse 3, 52072 Aachen, Deutchland
***University of Belgrade, Technical Faculty Bor, VJ 12, 19210 Bor, Serbia

Dedicated to Prof. Ing. Jaroslav Šesták, DrSc. at the occasion of his 70th birthday

(Received 10 October 2008; accepted 16 October 2008)

Abstract

Thermodynamic calculations of three binary Ti-based alloys: Ti-Al, Ti-Fe, and Al-Fe, as well as ternary alloy Ti-Al-Fe, is shown in this paper. Thermodynamic calculations involved thermodynamic determination of activities, coefficient of activities, partial and integral values for enthalpies and Gibbs energies of mixing and excess energies at different temperatures: 1873K, 2000K and 2073K, as well as calculated phase diagrams for the investigated binary and ternary systems. The FactSage is used for all thermodynamic calculations.

Keywords: Alloys, Ti-Al, Ti-Fe, Al-Fe, Ti-Al-Fe, thermodynamic calculations

1. Introduction

Last few years a lot of binary and multicomponent innovative iron aluminium alloys were developed: Fe-Al, Fe-Ga, Al-Fe-Ni, Fe-Ni-Ti, Fe-Al-Ni-Zr, Ni-Cr-Al-W, Al-Fe-Ni-Ti and Fe-Al-Ni-Cr [1]. The main reason for this huge scientific attention is certainly the large applications of these alloys, especially in the aerospace industry, due to their high oxidation resistance, low density and high melting point.

The Ti-Al-Fe-based alloys, which are thermodynamically investigated in this paper, belong to the group of alloyed aluminides and have not been completely reported in literature.

Due to the combination of light weight

* *Corresponding author: anakostov@ibb-bor.co.yu, kostov2004@yahoo.com*

DOI:10.2298/JMMB0801049K

and high strength, Ti-Al-Fe alloys are of practical interest for aerospace and automotive industries, as well as for various high temperature applications. Since the alloys with lower content of aluminium are brittle and provide moderate resistance to oxidation, alloying with the third elements enhances their ductility, strength, oxidation, and corrosion resistance.

There are a few thermodynamic studies in world literature. The most are based on thermodynamics and CALPHAD approach.

Thermodynamic properties of molten Al–Mn, Al–Cu and Al–Fe–Cu alloys in a temperature range of 1123–1878 K have been studied by Zaitsev et al [2] using the integral effusion method and Knudsen mass spectrometry. Thermodynamic functions of melts were described by the associated solution model.

Phase diagrams of the Fe-binary based systems had also a lot of scientific attention by different authors [3-6].

A lot of authors were investigated thermodynamic assessment of different iron-aluminides. Liu and Chang [7] have been analyzed thermodynamics of the Al-Fe-Si system as well as Ikeda et al [8] phase equilibria and stability of ordered BCC phases in the Fe-rich portion of the Fe3Al system. Thermodynamic assessment of the quaternary system Al-Fe-Mn-Si in the Al-rich corner was studied by Balitchev et al [9]. Thermodynamic description of the Cu-Al-Fe system at the Cu-Fe side has been given by Miettinen [10]. Thermodynamics of the Fe-Al-C ternary system has been investigated by incorporating ab initio energetic calculations into the CALPHAD approach by Ohtani et al [11].

Ti-Al-based alloys were one of the first materials types to which thermodynamic phase diagram calculation were applied. However, the early limitations in modelling, particularly with respect to the uptake of elements such as oxygen and nitrogen, restricted their use [12]. The first detailed presentation on thermodynamic phase diagram calculations for titanium alloys was made by Kaufman and Nesor [13] at the 2nd World Conference on Titanium. They presented a series of computer calculated phase diagrams for Ti-based alloys and even included an early calculation for the Ti-Al system. Since then substantial advances have been made in terms of theoretical models, computer software and hardware and it is now possible to deal with extremely complex materials on a routine basis [12].

Ti-Al-based alloys have been also studied by Kostov et al [14-19].

It can be anticipated that most of the thermodynamic data of ternary and multi-component high temperature systems come from theoretical calculations, rather than from direct experimentation. The main reasons are experimental difficulties, especially high investigation temperatures required. The similar situation is typical for Ti-Al-Fe system. The aim of this paper is to give a thermodynamic contribution the Ti-Al-Fe ternary system and its binary systems in the liquid phase using FactSage Thermo-chemical Software and Database [20], as well as to show the possibility of application of the used software in thermodynamic description of investigated systems.

2. Results and Discussion

Thermodynamic calculations in Ti-Al, Ti-Fe, Al-Fe and Ti-Al-Fe systems has been done using FactSage Thermo-chemical Software and Database [20]. The FactSage

package consists of a series of information, database, calculation and manipulation modules that enable one to access and manipulate pure substances and solution databases. The reaction, equilib, phase diagram and figure modules was used in this paper.

The results of calculated activities in binary systems Ti-Al, Ti-Fe, Al-Fe at 1873K, 2000K and 2073K are presented in figures 1, 2 and 3, respectively. Integral Gibbs energy of mixing and integral excess Gibbs energy for the investigated binary system are shown in figures 3-5.

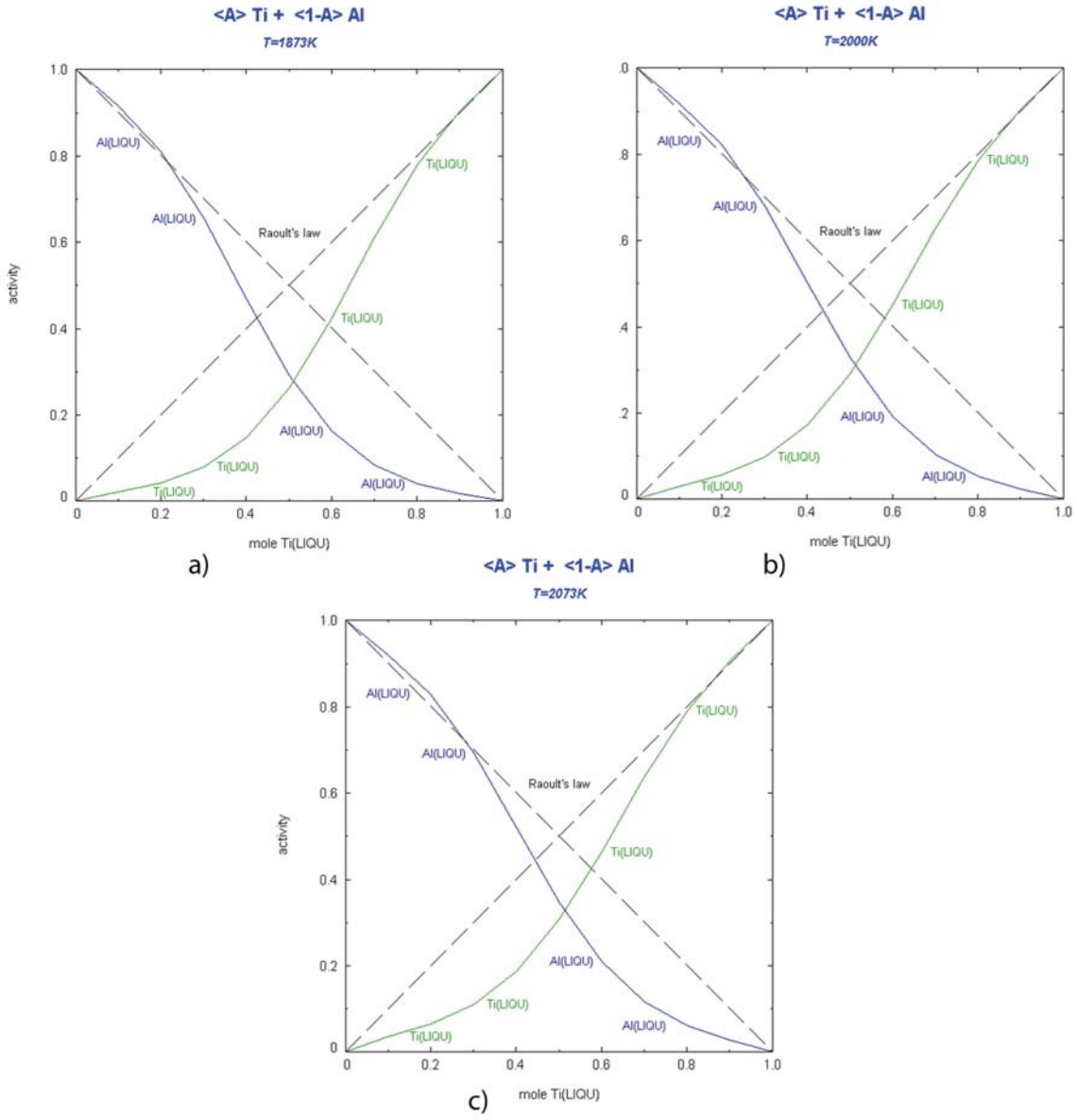

Fig.1. Activity of titanium and aluminium in Ti-Al system at different temperatures a) 1873K, b) 2000K, c) 2073K

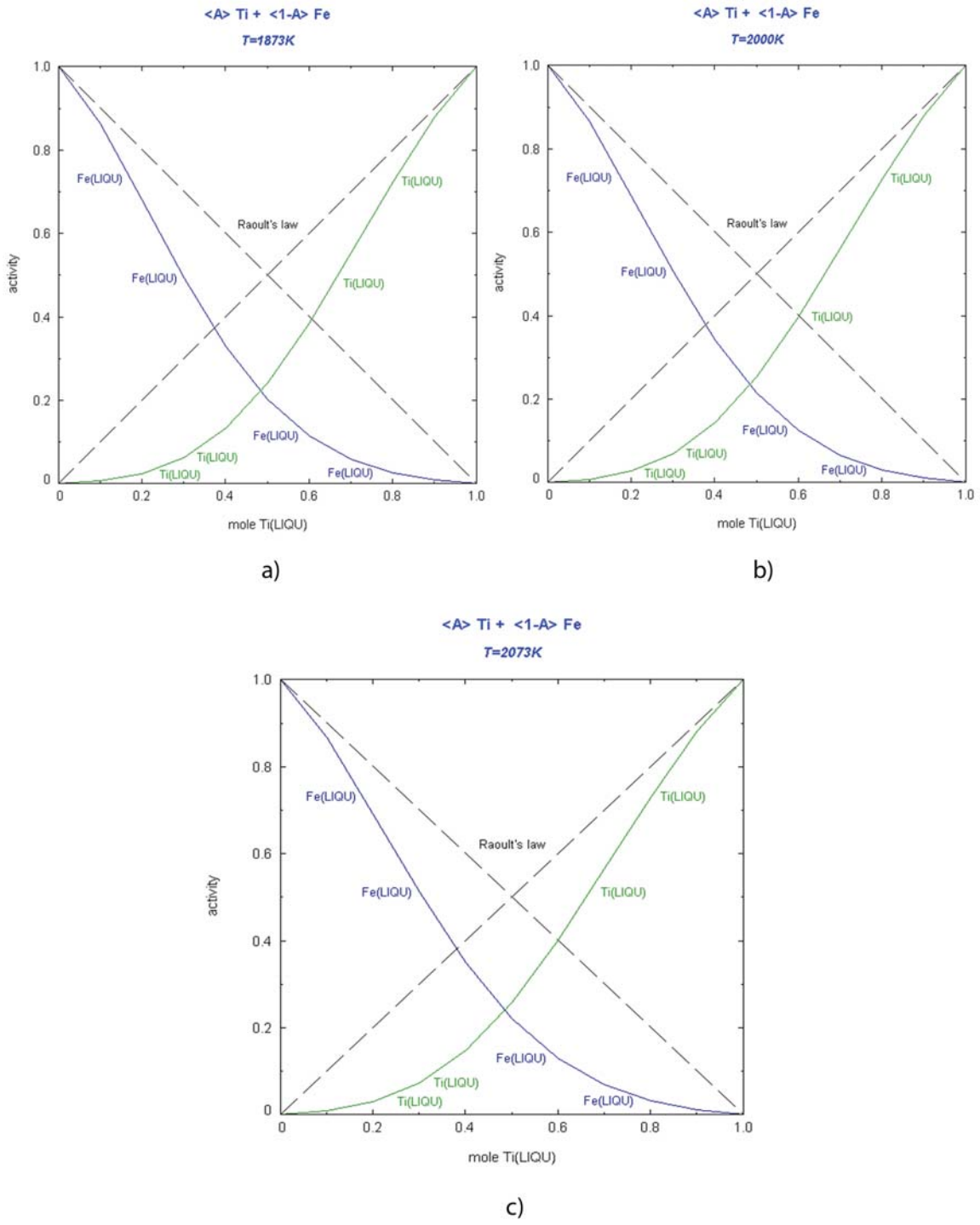

Fig.2. Activity of titanium and iron in Ti-Fe system at different temperatures a) 1873K, b) 2000K, c) 2073K

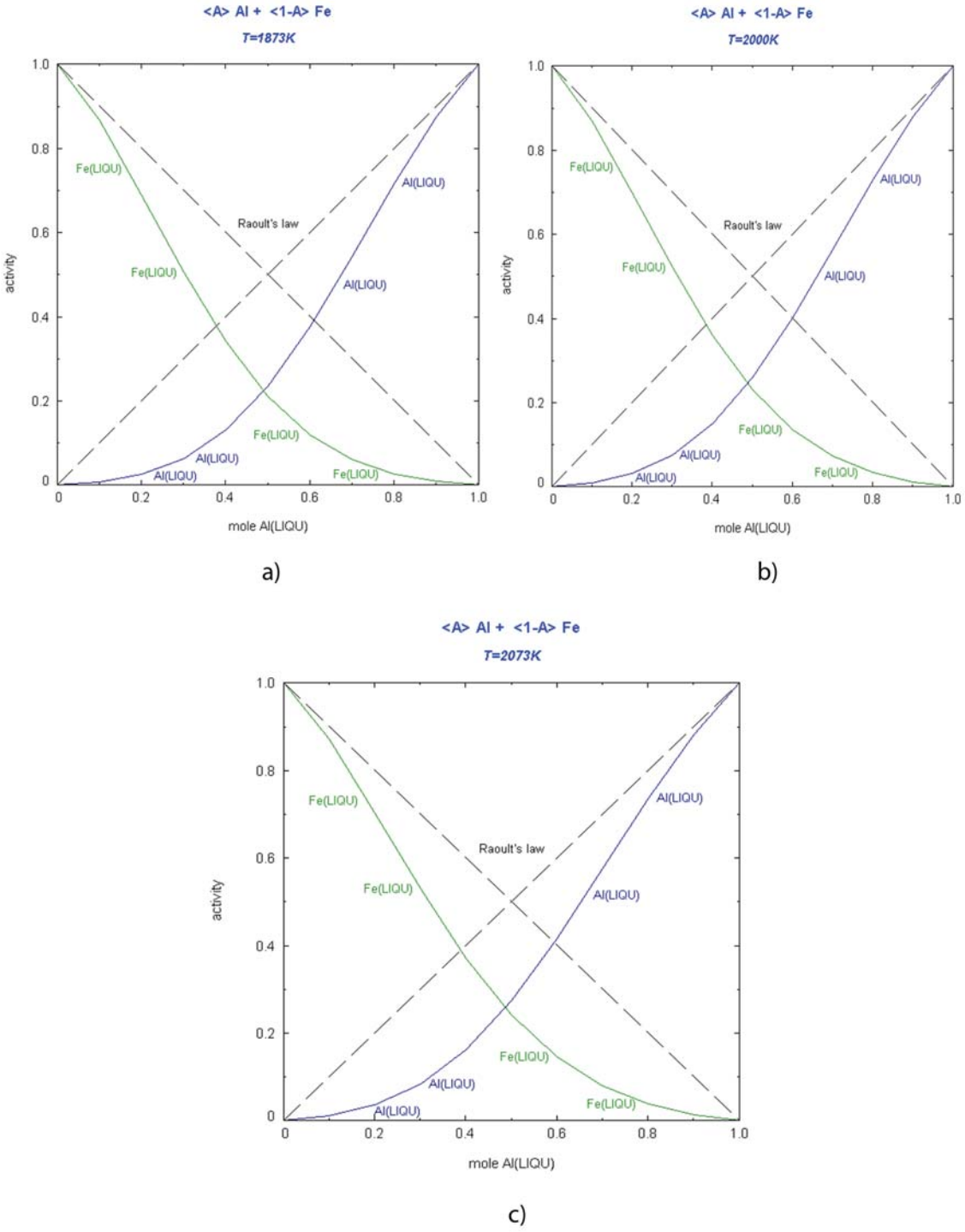

Fig.3. Activity of aluminium and iron in Al-Fe system at different temperatures a) 1873K, b) 2000K, c) 2073K

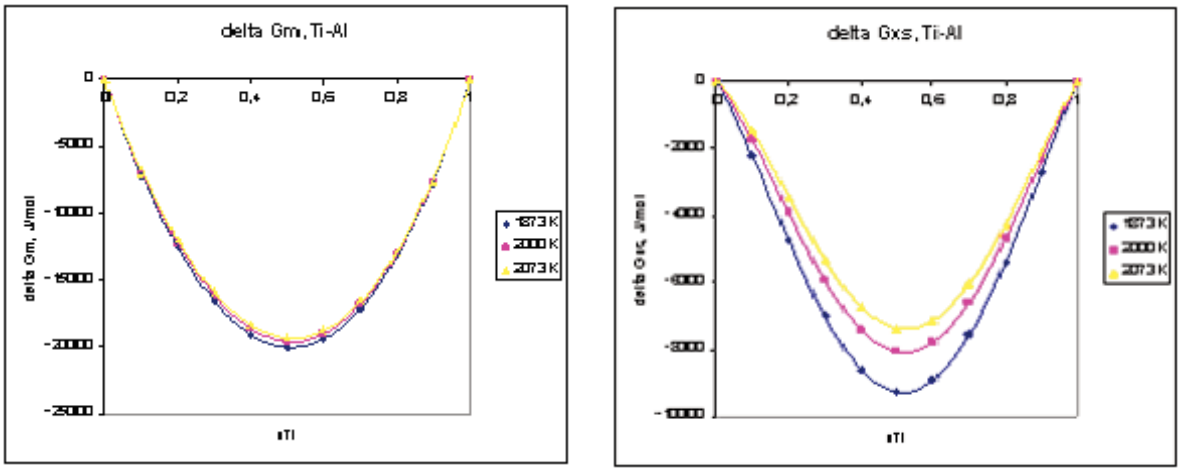

Fig.4. Integral Gibbs energy of mixing and integral excess Gibbs energy for Ti-Al binary system

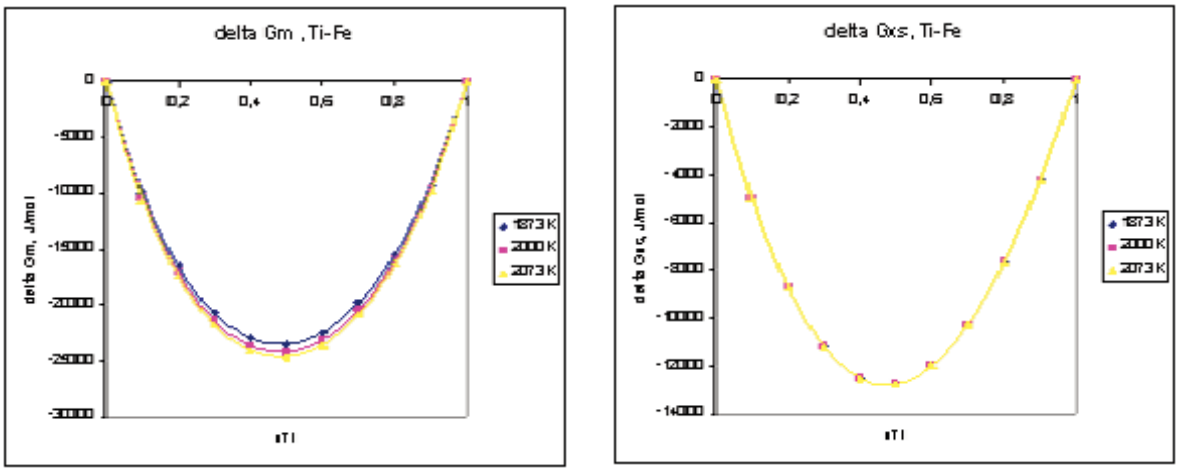

Fig.5. Integral Gibbs energy of mixing and integral excess Gibbs energy for Ti-Fe binary system

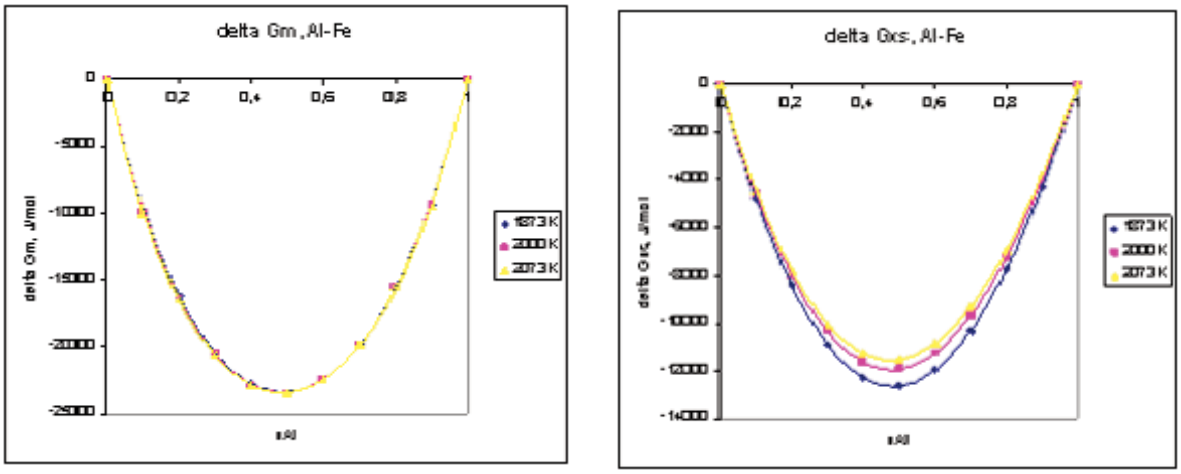

Fig.6. Integral Gibbs energy of mixing and integral excess Gibbs energy for Al-Fe binary system

Strong negative deviation from ideal behaviour can be noticed for liquid Ti-Al, Ti-Fe and Al-Fe alloys. The activities increase proportionally with increasing of the temperature. The activity and coefficient of activity values of the investigated components showed characteristics according to the Raoult's law. Considering calculated integral thermodynamic properties, all constitutive binary systems show negative values for integral Gibbs energy of mixing and integral excess Gibbs energy.

Phase diagrams of the investigated binary systems obtained by FactSage are shown in Figs. 7, 8 and 9, respectively. Comparison with referent data [6] indicate to fairly well accordance with available phase diagrams in literature.

Thermodynamic investigations of Ti-Al-Fe ternary system were carried out from each corner using 15 cross sections in total. The compositions of all investigated cross sections are given in Table 1.

Table 1. Composition of Ti-Al-Fe ternary alloys in the investigated sections

Cross section	A	B	C	D	E
$x_{Al} : x_{Fe}$	9:01	7:03	5:05	3:07	1:09
$x_{Ti} : x_{Fe}$	9:01	7:03	5:05	3:07	1:09
$x_{Ti} : x_{Al}$	9:01	7:03	5:05	3:07	1:09

Activity values in the investigated Ti-Al-Fe ternary system at 1873K, 2000K and 2073K are given in Tables 2, 3 and 4.

Activity values for titanium, aluminium and iron equally increasing with the

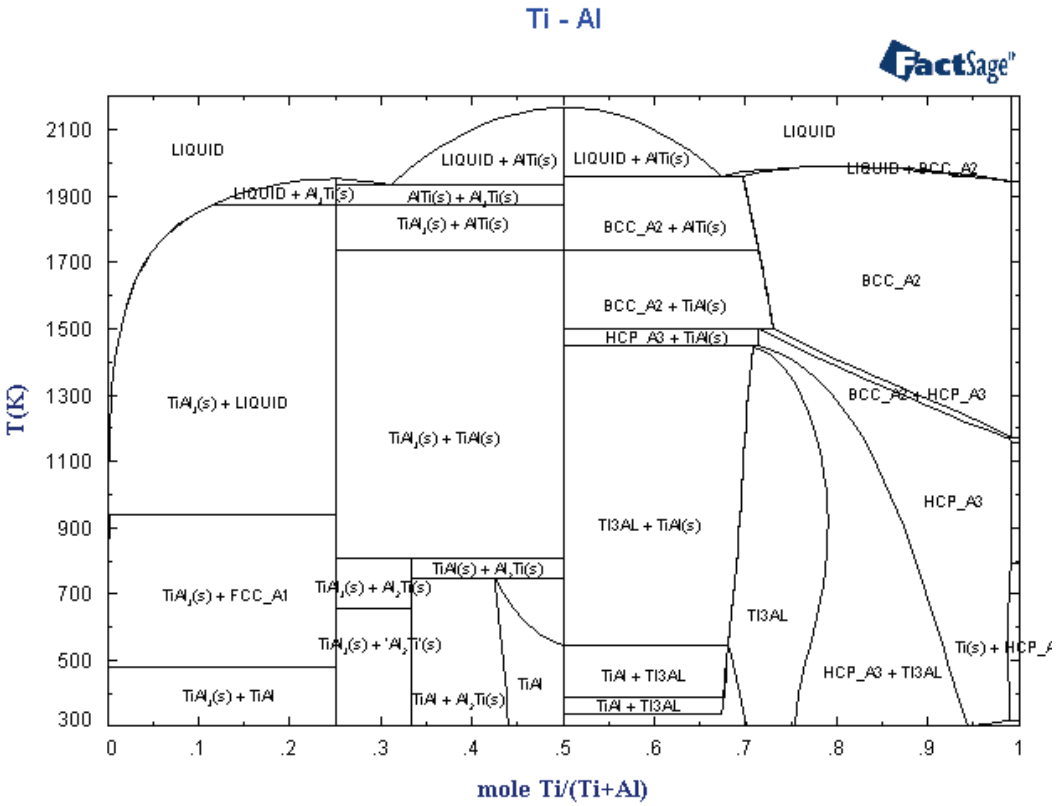

Fig.7. Phase diagram of Ti-Al system

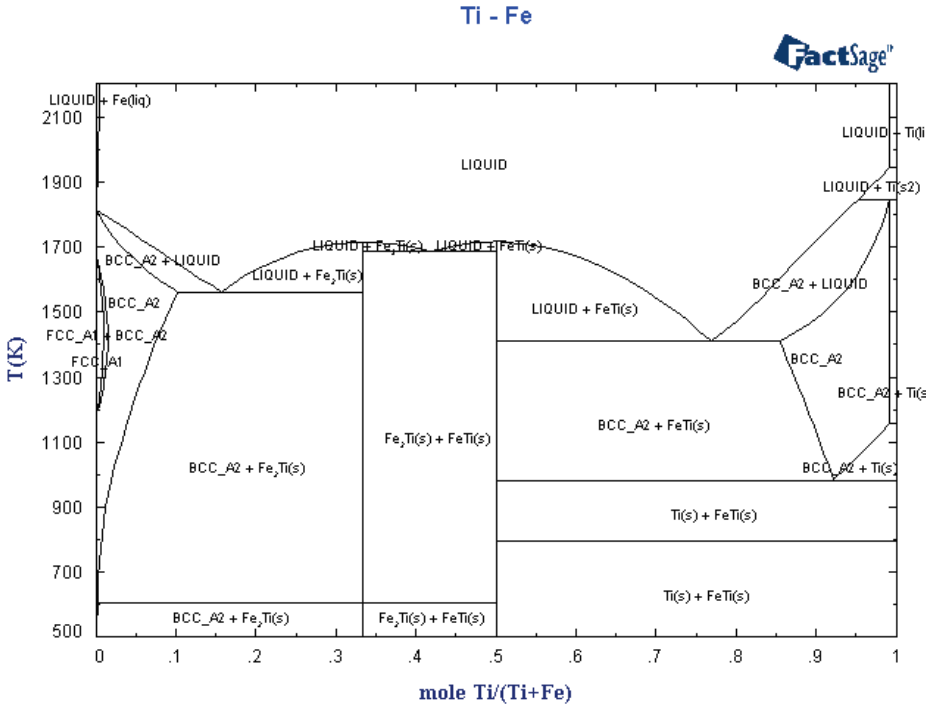

Fig.9. Phase diagram of Al-Fe system

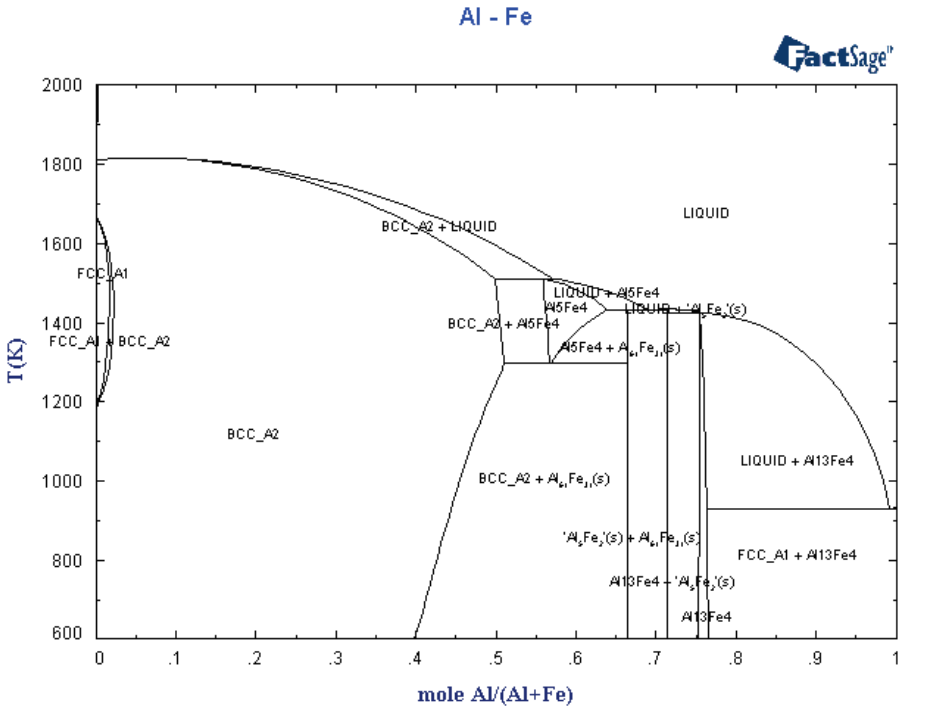

Fig.8. Phase diagram of Ti-Fe system

Table 2. Activity of the components at 1873K for Ti-Al-Fe ternary system

x_{Ti}	x_{Al}	x_{Fe}	a_{Ti}	a_{Al}	a_{Fe}	x_{Al}	x_{Fe}	a_{Ti}	a_{Al}	a_{Fe}
Cross section A						Cross section B				
0	0.9	0.1	0	0.877	0.008	0.7	0.3	0	0.542	0.060
0.1	0.81	0.09	0.021	0.798	0.007	0.63	0.27	0.022	0.497	0.051
0.2	0.72	0.08	0.047	0.691	0.007	0.56	0.24	0.054	0.422	0.044
0.3	0.63	0.07	0.090	0.543	0.006	0.49	0.21	0.107	0.327	0.037
0.4	0.54	0.06	0.165	0.381	0.006	0.42	0.18	0.193	0.229	0.030
0.5	0.45	0.05	0.284	0.238	0.005	0.35	0.15	0.315	0.147	0.022
0.6	0.36	0.04	0.443	0.134	0.004	0.28	0.12	0.469	0.087	0.015
0.7	0.27	0.03	0.621	0.070	0.002	0.21	0.09	0.633	0.049	0.009
0.8	0.18	0.02	0.782	0.035	0.001	0.14	0.06	0.781	0.026	0.005
0.9	0.09	0.01	0.903	0.015	0.001	0.07	0.03	0.901	0.012	0.002
1	0	0	1	0	0	0	0	1	0	0
Cross section C						Cross section D				
0	0.5	0.5	0	0.235	0.210	0.3	0.7	0	0.062	0.505
0.1	0.45	0.45	0.019	0.225	0.172	0.27	0.63	0.145	0.066	0.408
0.2	0.4	0.4	0.054	0.197	0.138	0.24	0.56	0.045	0.064	0.313
0.3	0.35	0.35	0.112	0.158	0.106	0.21	0.49	0.101	0.056	0.226
0.4	0.3	0.3	0.201	0.117	0.076	0.18	0.42	0.187	0.046	0.153
0.5	0.25	0.25	0.324	0.080	0.051	0.15	0.35	0.306	0.035	0.097
0.6	0.2	0.2	0.472	0.052	0.032	0.12	0.28	0.451	0.025	0.057
0.7	0.15	0.15	0.628	0.032	0.018	0.09	0.21	0.608	0.017	0.030
0.8	0.1	0.1	0.773	0.018	0.009	0.06	0.14	0.758	0.011	0.014
0.9	0.05	0.05	0.896	0.009	0.003	0.03	0.07	0.890	0.005	0.005
1	0	0	1	0	0	0	0	1	0	0
Cross section E										
0	0.1	0.9	0	0.006	0.867					
0.1	0.09	0.81	0.009	0.008	0.721					
0.2	0.08	0.72	0.031	0.009	0.555					
0.3	0.07	0.63	0.077	0.010	0.396					
0.4	0.06	0.54	0.154	0.009	0.263					
0.5	0.05	0.45	0.267	0.008	0.162					
0.6	0.04	0.36	0.411	0.007	0.092					
0.7	0.03	0.27	0.573	0.005	0.048					
0.8	0.02	0.18	0.737	0.003	0.021					
0.9	0.01	0.09	0.883	0.002	0.007					
1	0	0	1	0	0					

Table 3. Activity of the components at 2000K for Ti-Al-Fe ternary system

x_{Ti}	x_{Al}	x_{Fe}	a_{Ti}	a_{Al}	a_{Fe}	x_{Al}	x_{Fe}	a_{Ti}	a_{Al}	a_{Fe}
Cross section A						Cross section B				
0	0.9	0.1	0	0.880	0.011	0.7	0.3	0	0.563	0.072
0.1	0.81	0.09	0.029	0.808	0.009	0.63	0.27	0.028	0.523	0.059
0.2	0.72	0.08	0.060	0.710	0.008	0.56	0.24	0.065	0.453	0.051
0.3	0.63	0.07	0.109	0.573	0.008	0.49	0.21	0.124	0.360	0.042
0.4	0.54	0.06	0.189	0.417	0.007	0.42	0.18	0.213	0.262	0.034
0.5	0.45	0.05	0.310	0.272	0.006	0.35	0.15	0.336	0.175	0.025
0.6	0.36	0.04	0.466	0.161	0.004	0.28	0.12	0.486	0.109	0.017
0.7	0.27	0.03	0.636	0.089	0.003	0.21	0.09	0.644	0.064	0.010
0.8	0.18	0.02	0.788	0.047	0.002	0.14	0.06	0.786	0.036	0.005
0.9	0.09	0.01	0.905	0.021	0.001	0.07	0.03	0.901	0.017	0.002
1	0	0	1	0	0	0	0	1	0	0
Cross section C						Cross section D				
0	0.5	0.5	0	0.259	0.230	0.3	0.7	0	0.075	0.520
0.1	0.45	0.45	0.024	0.251	0.187	0.27	0.63	0.017	0.080	0.421
0.2	0.4	0.4	0.062	0.224	0.149	0.24	0.56	0.052	0.078	0.325
0.3	0.35	0.35	0.125	0.185	0.115	0.21	0.49	0.111	0.070	0.237
0.4	0.3	0.3	0.217	0.140	0.083	0.18	0.42	0.200	0.059	0.163
0.5	0.25	0.25	0.340	0.099	0.056	0.15	0.35	0.319	0.046	0.105
0.6	0.2	0.2	0.485	0.066	0.035	0.12	0.28	0.462	0.034	0.063
0.7	0.15	0.15	0.636	0.042	0.020	0.09	0.21	0.615	0.023	0.034
0.8	0.1	0.1	0.777	0.025	0.010	0.06	0.14	0.762	0.015	0.017
0.9	0.05	0.05	0.897	0.012	0.004	0.03	0.07	0.891	0.008	0.006
1	0	0	1	0	0	0	0	1	0	0
Cross section E										
0	0.1	0.9	0	0.009	0.869					
0.1	0.09	0.81	0.010	0.011	0.726					
0.2	0.08	0.72	0.035	0.013	0.563					
0.3	0.07	0.63	0.084	0.013	0.407					
0.4	0.06	0.54	0.164	0.013	0.274					
0.5	0.05	0.45	0.278	0.011	0.172					
0.6	0.04	0.36	0.421	0.009	0.100					
0.7	0.03	0.27	0.581	0.007	0.053					
0.8	0.02	0.18	0.741	0.005	0.025					
0.9	0.01	0.09	0.884	0.003	0.008					
1	0	0	1	0	0					

Table 4. Activity of the components at 2073K for Ti-Al-Fe ternary system

x_{Ti}	x_{Al}	x_{Fe}	a_{Ti}	a_{Al}	a_{Fe}	x_{Al}	x_{Fe}	a_{Ti}	a_{Al}	a_{Fe}
Cross section A						Cross section B				
0	0.9	0.1	0	0.882	0.013	0.7	0.3	0	0.574	0.079
0.1	0.81	0.09	0.034	0.813	0.011	0.63	0.27	0.031	0.536	0.065
0.2	0.72	0.08	0.068	0.720	0.010	0.56	0.24	0.072	0.470	0.055
0.3	0.63	0.07	0.120	0.589	0.009	0.49	0.21	0.133	0.379	0.045
0.4	0.54	0.06	0.203	0.437	0.008	0.42	0.18	0.224	0.281	0.036
0.5	0.45	0.05	0.324	0.291	0.006	0.35	0.15	0.347	0.192	0.026
0.6	0.36	0.04	0.479	0.178	0.005	0.28	0.12	0.495	0.122	0.018
0.7	0.27	0.03	0.644	0.101	0.003	0.21	0.09	0.649	0.073	0.011
0.8	0.18	0.02	0.792	0.054	0.002	0.14	0.06	0.789	0.042	0.006
0.9	0.09	0.01	0.905	0.025	0.001	0.07	0.03	0.902	0.020	0.002
1	0	0	1	0	0	0	0	1	0	0
Cross section C						Cross section D				
0	0.5	0.5	0	0.273	0.240	0.3	0.7	0	0.083	0.528
0.1	0.45	0.45	0.026	0.266	0.195	0.27	0.63	0.019	0.089	0.428
0.2	0.4	0.4	0.067	0.240	0.155	0.24	0.56	0.055	0.087	0.331
0.3	0.35	0.35	0.132	0.200	0.119	0.21	0.49	0.116	0.079	0.243
0.4	0.3	0.3	0.226	0.154	0.087	0.18	0.42	0.207	0.066	0.168
0.5	0.25	0.25	0.349	0.111	0.059	0.15	0.35	0.327	0.053	0.109
0.6	0.2	0.2	0.492	0.076	0.038	0.12	0.28	0.468	0.039	0.066
0.7	0.15	0.15	0.641	0.049	0.022	0.09	0.21	0.619	0.027	0.036
0.8	0.1	0.1	0.779	0.030	0.011	0.06	0.14	0.764	0.018	0.018
0.9	0.05	0.05	0.897	0.015	0.004	0.03	0.07	0.892	0.009	0.007
1	0	0	1	0	0	0	0	1	0	0
Cross section E										
0	0.1	0.9	0	0.010	0.871					
0.1	0.09	0.81	0.011	0.013	0.728					
0.2	0.08	0.72	0.038	0.015	0.568					
0.3	0.07	0.63	0.088	0.015	0.413					
0.4	0.06	0.54	0.170	0.015	0.281					
0.5	0.05	0.45	0.285	0.013	0.178					
0.6	0.04	0.36	0.427	0.011	0.105					
0.7	0.03	0.27	0.585	0.009	0.056					
0.8	0.02	0.18	0.743	0.006	0.026					
0.9	0.01	0.09	0.885	0.003	0.009					
1	0	0	1	0	0					

Table 5. Integral Gibbs energy of mixing and excess Gibbs energy for Ti-Al-Fe ternary system at 1873K

x_{Ti}	x_{Al}	xFe	ΔG^M	ΔG^E	x_{Al}	x_{Fe}	ΔG^M	ΔG^E
Cross section A					Cross section B			
0	0,9	0,1	-9354	-4292	0,7	0,3	-19828	-10316
0,1	0,81	0,09	-15771	-6153	0,63	0,27	-25363	-11740
0,2	0,72	0,08	-19931	-8088	0,56	0,24	-28300	-12897
0,3	0,63	0,07	-22730	-9674	0,49	0,21	-29728	-13557
0,4	0,54	0,06	-24123	-10605	0,42	0,18	-29746	-13558
0,5	0,45	0,05	-24015	-10690	0,35	0,15	-28365	-12815
0,6	0,36	0,04	-22363	-9858	0,28	0,12	-25599	-11314
0,7	0,27	0,03	-19184	-8153	0,21	0,09	-21479	-9113
0,8	0,18	0,02	-14542	-5737	0,14	0,06	-16040	-6346
0,9	0,09	0,01	-8456	-2888	0,07	0,03	-9229	-3216
1	0	0	0	0	0	0	0	0
Cross section C					Cross section D			
0	0,5	0,5	-23425	-12631	0,3	0,7	-20408	-10896
0,1	0,45	0,45	-28921	-14144	0,27	0,63	-23210	-9586
0,2	0,4	0,4	-31543	-15115	0,24	0,56	-30043	-14641
0,3	0,35	0,35	-32512	-15444	0,21	0,49	-31465	-15294
0,4	0,3	0,3	-32029	-15073	0,18	0,42	-31326	-15138
0,5	0,25	0,25	-30175	-13984	0,15	0,35	-29751	-14201
0,6	0,2	0,2	-26999	-12201	0,12	0,28	-26812	-12527
0,7	0,15	0,15	-22538	-9787	0,09	0,21	-22546	-10180
0,8	0,1	0,1	-16797	-6846	0,06	0,14	-16935	-7240
0,9	0,05	0,05	-9664	-3522	0,03	0,07	-9821	-3808
1	0	0	0	0	0	0	0	0
Cross section E								
0	0,1	0,9	-9851	-4789				
0,1	0,09	0,81	-18257	-8639				
0,2	0,08	0,72	-23226	-11384				
0,3	0,07	0,63	-26125	-13069				
0,4	0,06	0,54	-27264	-13746				
0,5	0,05	0,45	-26794	-13470				
0,6	0,04	0,36	-24803	-12298				
0,7	0,03	0,27	-21327	-10296				
0,8	0,02	0,18	-16335	-7530				
0,9	0,01	0,09	-9641	-4072				
1	0	0	0	0				

Table 6. Integral Gibbs energy of mixing and excess Gibbs energy for Ti-Al-Fe ternary system at 2000K

x_{Ti}	x_{Al}	xFe	ΔG^M	ΔG^E	x_{Al}	x_{Fe}	ΔG^M	ΔG^E
Cross section A					Cross section B			
0	0.9	0.1	-9400	-3994	0.7	0.3	-19831	-9674
0.1	0.81	0.09	-15759	-5488	0.63	0.27	-25446	-10899
0.2	0.72	0.08	-19806	-7161	0.56	0.24	-28374	-11927
0.3	0.63	0.07	-22525	-8583	0.49	0.21	-29790	-12523
0.4	0.54	0.06	-23877	-9442	0.42	0.18	-29807	-12521
0.5	0.45	0.05	-23771	-9543	0.35	0.15	-28437	-11833
0.6	0.36	0.04	-22159	-8806	0.28	0.12	-25693	-10440
0.7	0.27	0.03	-19048	-7269	0.21	0.09	-21600	-8395
0.8	0.18	0.02	-14490	-5088	0.14	0.06	-16180	-5828
0.9	0.09	0.01	-8482	-2536	0.07	0.03	-9360	-2939
1	0	0	0	0	0	0	0	0
Cross section C					Cross section D			
0	0.5	0.5	-23454	-11928	0.3	0.7	-20515	-10358
0.1	0.45	0.45	-29127	-13348	0.27	0.63	-27146	-12599
0.2	0.4	0.4	-31811	-14269	0.24	0.56	-30504	-14057
0.3	0.35	0.35	-32815	-14590	0.21	0.49	-31990	-14722
0.4	0.3	0.3	-32355	-14248	0.18	0.42	-31885	-14599
0.5	0.25	0.25	-30514	-13225	0.15	0.35	-30319	-13715
0.6	0.2	0.2	-27341	-11540	0.12	0.28	-27364	-12111
0.7	0.15	0.15	-22869	-9254	0.09	0.21	-23053	-9848
0.8	0.1	0.1	-17093	-6468	0.06	0.14	-17360	-7008
0.9	0.05	0.05	-9880	-3322	0.03	0.07	-10108	-3687
1	0	0	0	0	0	0	0	0
Cross section E								
0	0.1	0.9	-9986	-4581				
0.1	0.09	0.81	-18693	-8423				
0.2	0.08	0.72	-23814	-11168				
0.3	0.07	0.63	-26803	-12862				
0.4	0.06	0.54	-27988	-13554				
0.5	0.05	0.45	-27527	-13298				
0.6	0.04	0.36	-25506	-12153				
0.7	0.03	0.27	-21961	-10182				
0.8	0.02	0.18	-16852	-7451				
0.9	0.01	0.09	-9978	-4032				
1	0	0	0	0				

Table 7. Integral Gibbs energy of mixing and excess Gibbs energy for Ti-Al-Fe ternary system at 2073K

x_{Ti}	x_{Al}	xFe	ΔG^M	ΔG^E	x_{Al}	x_{Fe}	ΔG^M	ΔG^E
Cross section A					Cross section B			
0	0,9	0,1	-9426	-3823	0,7	0,3	-19833	-9304
0,1	0,81	0,09	-15752	-5106	0,63	0,27	-25493	-10415
0,2	0,72	0,08	-19735	-6628	0,56	0,24	-28416	-11369
0,3	0,63	0,07	-22407	-7956	0,49	0,21	-29826	-11928
0,4	0,54	0,06	-23736	-8775	0,42	0,18	-29842	-11926
0,5	0,45	0,05	-23631	-8883	0,35	0,15	-28479	-11269
0,6	0,36	0,04	-22041	-8200	0,28	0,12	-25747	-9937
0,7	0,27	0,03	-18969	-6760	0,21	0,09	-21669	-7982
0,8	0,18	0,02	-14460	-4715	0,14	0,06	-16261	-5531
0,9	0,09	0,01	-8497	-2334	0,07	0,03	-9435	-2780
1	0	0	0	0	0	0	0	0
Cross section C					Cross section D			
0	0,5	0,5	-23471	-11525	0,3	0,7	-20577	-10048
0,1	0,45	0,45	-29245	-12890	0,27	0,63	-27347	-12269
0,2	0,4	0,4	-31964	-13783	0,24	0,56	-30769	-13722
0,3	0,35	0,35	-32989	-14099	0,21	0,49	-32291	-14393
0,4	0,3	0,3	-32542	-13775	0,18	0,42	-32206	-14290
0,5	0,25	0,25	-30708	-12789	0,15	0,35	-30646	-13435
0,6	0,2	0,2	-27538	-11160	0,12	0,28	-27682	-11871
0,7	0,15	0,15	-23060	-8948	0,09	0,21	-23345	-9658
0,8	0,1	0,1	-17263	-6250	0,06	0,14	-17604	-6874
0,9	0,05	0,05	-10005	-3207	0,03	0,07	-10272	-3617
1	0	0	0	0	0	0	0	0
Cross section E								
0	0,1	0,9	-10064	-4461				
0,1	0,09	0,81	-18944	-8299				
0,2	0,08	0,72	-24152	-11045				
0,3	0,07	0,63	-27193	-12743				
0,4	0,06	0,54	-28405	-13444				
0,5	0,05	0,45	-27948	-13200				
0,6	0,04	0,36	-25911	-12070				
0,7	0,03	0,27	-22325	-10116				
0,8	0,02	0,18	-17150	-7405				
0,9	0,01	0,09	-10171	-4008				
1	0	0	0	0				

component's content increasing. Activity of the three components is increasing per sections from A to E and with the temperature increasing, too and according to the Raoult's law.

Values for the integral Gibbs energy of mixing and integral excess Gibbs energy of Ti-Al-Fe ternary system at 1873K, 2000K and 2073K are presented in Tables 5, 6 and 7.

The enthalpies of mixing values indicate that the strongest chemical interaction between the components in the investigated Ti-Al-Fe ternary system exists between aluminium and iron and the weakest between titanium and iron. In the case of investigated sections from aluminium corner, these values are strongly affected by Ti-Fe binary system.

3. Conclusions

The thermodynamic calculations in binary alloys Ti-Al, Ti-Fe and Al-Fe, as well as ternary Ti-Al-Fe at 1873K, 2000K and 2073K were determined. All three investigated binary systems have negative values for integral Gibbs mixing energy and integral excess Gibbs energy. Activity values of the components are less than unity and show negative deviation from the Raoult's law. Phase diagrams for the investigated binary systems are calculated by the use of Fact Sage.

Providing in mind that no experimental data for these systems have been done or reported, obtained results presented one good base for the further thermodynamic analysis and developing in these group of innovative iron aluminum alloys.

The obtained and shown results for the Ti-Al-Fe-based system provide complete thermodynamic determination optimization of this investigated system.

Acknowledgements

First author would like to thank the Alexander von Humboldt Foundation, Bonn, Germany, for supporting and sponsoring this research work at the IME Institute for Process Metallurgy and Metal Recycling, RWTH Aachen, Germany.

References:

1.Final Conference COST Action 535 Thermodynamics of Alloyed Aluminides (THALU), 4th Discussion Meeting on the Development of Innovative Iron Aluminum Alloys, 21 – 24 October 2007, Interlaken, Switzerland.

2. A.I.Zaitsev, N.E. Zaitseva, N.E. Shimko, N.A. Artyunyan, S.F. Dunaev, V.S. Kraposhin, L. Ha Thanh, *J. Phys.: Condens. Matter.*, 20 (2008) 114-121.

3. M. Seiersten , unpublished work (1989), Available in SSOL2 and BIN database.

4. U.R. Kattner, B.P. Burton, Phase Diagrams of Binary Iron Alloys, (Ed.) H. Okamoto, ASM International, Materials Park, OH, (1993) pp. 12-28.

5. M. Seiersten, COST 507, Thermochemical database for light metal alloys, Vol.2, (Ed.) I.Ansara, A.T.Dinsdale, M.H.Rand, (1998), Available in COST2 database.

6. B. Predel, Numerical Data and Functional Relationships in Science and Technology, in Landolt-Börnstein - Group IV Physical Chemistry, Volume 5a, (Ed.) Springer-Verlag, 2006, ISSN 1615-2018.

7. Z.-K. Liu, Y.A.Chang, *Metall. Mater. Trans. A*, 30A (1999) 1081-1095.

8. O. Ikeda, I. Ohnuma, R. Kainuma, K.

Ishida, *Intermetallics*, 9 (2001) 755-761.

9. E. Balitchev, T. Jantzen, I. Hurtado, D. Neuschutz, *CALPHAD,* 27 (2003) 275-278.

10. J. Miettinen, *CALPHAD*, 27 (2003) 91-102.

11. H. Ohtani, M.Yamano, M. Hasebe, *ISIJ Int.*, 44 (2004) 1738-1747.

12. N. Saunders, Titanium '95: Science and Technology, eds. P. Bleckinsop, W.J. Evans and H.M. Flower, Institute of Materials, London, 1996, p.2167.

13. L. Kaufman, N. Nesor, *CALPHAD*, 2 (1978) 325.

14. A. Kostov, B. Friedrich, D. Zivkovic, *Computational Materials Science*, Vol.37, 3 (2006) 355-360.

15. A. Kostov, D. Zivkovic, B. Friedrich, *Journal of Mining and Metallurgy*, 42B (2006) 57-65.

16. A. Kostov, D. Zivkovic, B. Friedrich, *Journal of Mining and Metallurgy*, 43B (2007) 29-38.

17. D. Zivkovic, A. Kostov, I. Katayama, D. Manasijevic, N. Strbac, *Materials at High Temperatures*, 24 (1) (2007) 37.

18. A. Kostov, D. Zivkovic, *J. Serb. Chem. Soc.*, 73 (4) 499-506 (2008).

19. A. Kostov, D. Zivkovic, *J. Alloys Compd.* 460 (2008) 164.

20. C.W. Bale, P. Chartrand, S.A. Degterov, G. Eriksson, K. Hack, R.B. Mahfoud, J. Melancon, A.D. Pelton, S. Petersen, *CALPHAD,* 26 (2) 2002, p.189.