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CALCULATION OF THERMODYNAMIC PROPERTIES OF Al-Fe, Al-Ni AND Ni-Fe ALLOYS USING FACTSAGE

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ABSTRACT
Thermodynamic predicting analysis of three binary systems Al-Fe, Al-Ni and Ni-Fe are shown in this paper. Thermodynamic analysis involved calculation of activities, coefficient of activities, partial and integral values for enthalpies and Gibbs energies of mixing and excess energies at three different temperatures: 1873K, 1900K and 1973K, as well as calculated phase diagrams, for the investigated binaries. The FactSage programme was used for all thermodynamic calculations.
Keywords: Al-Fe, Al-Ni, Ni-Fe, FactSage, thermodynamic predicting

1. INTRODUCTION
Intermetallic compounds have been considered recently as potential candidates for use as materials for high temperature applications. Many of the compounds of interest involve aluminum as the main component, and are known as aluminides. The motivation for introducing these new materials is that engines made of them can save natural resources, as they live longer and can reduce fuel consumption as they are lighter [1]. Compounds may become real engineering materials after further alloying to improve their in-service properties, e.g. mechanical properties or corrosion resistance. For example, a thorough knowledge of the phase equilibria and thermodynamic properties of the Al–Fe–Ni based system is of fundamental importance in many applications, such as Ni-base superalloys and Ni-base shape-memory alloys because of their good magnetic properties and high thermal stability [2].
Over the last decade, intense research has been conducted worldwide, to find other compounds exhibiting improved properties or having specific capabilities. Similarly, attempts have been made to find stable second phase particles, to improve high temperature stability and strength of potential industrial variants of Fe-Al and Ni-Al alloys; alloying is as necessary for the enhancement of the properties of intermetallic compounds as it is for any other metallic material. It should be stressed that the permutations for alloying combinations are endless. Thus, many new engineering materials can result from adding alloying additions to binary compounds.
Most of the modeling work made use of the so-called CALPHAD (CALculation of PHAse Diagrams) procedure that describes the Gibbs energy of any phase by means of parametric polynomial functions of composition and temperature considering all related experimental data available [1].
To the best of our knowledge, no thermodynamic modeling has been performed over the entire temperature and composition ranges for the Al–Fe–Ni based system so far. The purposes of the present work are: to briefly evaluate the measured phase diagram and thermodynamic data available

for the Al–Fe–Ni based binary systems, and to obtain an optimal set of thermodynamic parameters for the investigated systems over the whole composition and the selected temperature ranges.

2. RESULTS

Thermodynamic calculations in Al-Fe, Al-Ni and Ni-Fe binary systems have been done using FactSage [3]. The reactions, phase equilibria, phase diagram and figure modules was used in this paper.

Phase diagrams of the investigated binary systems obtained by FactSage are shown in Figs. 1, 2 and 3, respectively. Comparison with referent data [4] indicate to fairly well accordance with available phase diagrams in literature.

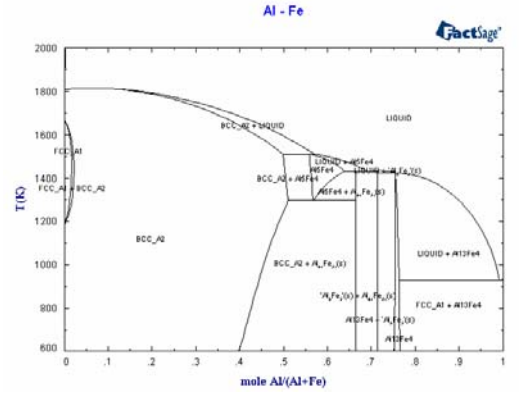

Figure 1. Phase diagram of Al-Fe system.

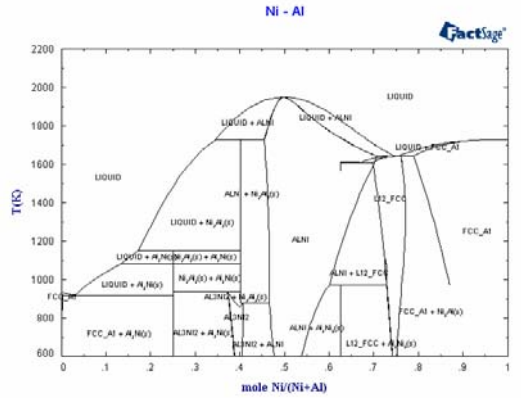

Figure 2. Phase diagram of Al-Ni system.

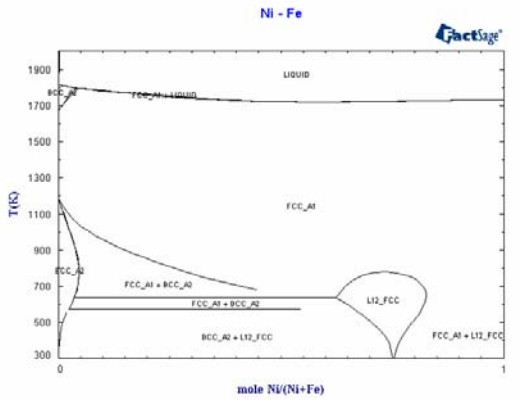

Figure 3. Phase diagram of Ni-Fe binary system.

The results of calculated activities, coefficient of activities, partial and integral values for enthalpies and Gibbs energies of mixing and excess energies at three different temperatures: 1873K, 1900K and 1973K for the investigated binary systems are given in Tables 1-3.

Strong negative deviation from ideal behavior can be noticed for liquid Al-Fe, Al-Ni and Ni-Fe systems. 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.

Table 1. Thermodynamic properties of Al-Fe binary system at 1873, 1900 and 1973 K.

X_{Al}	X_{Fe}	a_{Al}	a_{Fe}	γ_{Al}	γ_{Fe}	Gm Al	Gm Fe	Gxs Al	Gxs Fe	ΔGm	ΔGxs
1873 K											
0	1	0	1		1		0		0	0	0
0,1	0,9	0,006	0,866	0,064	0,962	-78426	-2232	-42570	-591	-9851	-4789
0,2	0,8	0,024	0,689	0,121	0,861	-57848	-5789	-32786	-2314	-16201	-8408
0,3	0,7	0,062	0,504	0,208	0,721	-43185	-10647	-24437	-5093	-20408	-10896
0,4	0,6	0,130	0,339	0,326	0,566	-31723	-16802	-17455	-8848	-22771	-12290
0,5	0,5	0,234	0,210	0,469	0,420	-22561	-24288	-11767	-13495	-23425	-12631
0,6	0,4	0,375	0,118	0,625	0,296	-15255	-33215	-7300	-18946	-22439	-11958
0,7	0,3	0,542	0,059	0,774	0,199	-9528	-43862	-3974	-25114	-19828	-10316
0,8	0,2	0,717	0,025	0,896	0,128	-5181	-56964	-1706	-31902	-15538	-7745
0,9	0,1	0,876	0,008	0,973	0,080	-2052	-75069	-412	-39213	-9354	-4292
1	0	1	0	1	0	0		0		0	0
1900 K											
0	1	0	1		1		0		0	0	0
0,1	0,9	0,006	0,867	0,069	0,963	-78523	-2253	-42150	-589	-9880	-4745
0,2	0,8	0,025	0,691	0,128	0,864	-57843	-5827	-32420	-2302	-16230	-8325
0,3	0,7	0,065	0,508	0,217	0,725	-43150	-10695	-24131	-5061	-20431	-10782
0,4	0,6	0,134	0,344	0,336	0,573	-31686	-16851	-17211	-8782	-22785	-12153
0,5	0,5	0,240	0,214	0,480	0,428	-22534	-24327	-11585	-13378	-23431	-12481
0,6	0,4	0,380	0,121	0,634	0,304	-15244	-33234	-7175	-18759	-22440	-11809
0,7	0,3	0,546	0,062	0,781	0,207	-9533	-43852	-3899	-24834	-19829	-10179
0,8	0,2	0,719	0,027	0,899	0,136	-5196	-56926	-1671	-31502	-15542	-7637
0,9	0,1	0,877	0,008	0,974	0,086	-2067	-75038	-402	-38665	-9364	-4228
1	0	1	0	1	0	0		0		0	0
1973 K											
0	1	0	1		1		0		0	0	0
0,1	0,9	0,008	0,868	0,082	0,965	-78785	-2310	-41014	-582	-9957	-4625
0,2	0,8	0,029	0,696	0,147	0,870	-57832	-5929	-31432	-2269	-16310	-8101
0,3	0,7	0,072	0,516	0,241	0,738	-43054	-10823	-23304	-4973	-20493	-10472
0,4	0,6	0,145	0,355	0,364	0,591	-31582	-16982	-16552	-8602	-22822	-11782
0,5	0,5	0,254	0,225	0,508	0,450	-22462	-24433	-11092	-13063	-23448	-12078
0,6	0,4	0,395	0,131	0,659	0,328	-15216	-33285	-6837	-18255	-22444	-11404
0,7	0,3	0,558	0,069	0,798	0,230	-9546	-43826	-3696	-24077	-19830	-9810
0,8	0,2	0,726	0,031	0,908	0,156	-5235	-56823	-1575	-30423	-15553	-7344
0,9	0,1	0,879	0,010	0,977	0,103	-2105	-74953	-377	-37183	-9390	-4057
1	0	1	0	1	0	0		0		0	0

Table 2. Thermodynamic properties of Al-Ni binary system at 1873, 1900 and 1973 K.

X_{Al}	X_{Ni}	a_{Al}	a_{Ni}	γ_{Al}	γ_{Ni}	Gm Al	Gm Ni	Gxs Al	Gxs Ni	ΔGm	ΔGxs
1873 K											
0	1	0	1		1		0		0	0	0
0,1	0,9	0,00016	0,874	0,001	0,971	-135753	-2090	-99897	-449	-15456	-10394
0,2	0,8	0,00084	0,654	0,004	0,817	-110227	-6607	-85165	-3132	-27331	-19539
0,3	0,7	0,0040528	0,386	0,013	0,552	-85777	-14790	-67029	-9236	-36086	-26574
0,4	0,6	0,017	0,175	0,043	0,292	-62977	-27091	-48708	-19136	-41445	-30965
0,5	0,5	0,063	0,061	0,126	0,123	-43021	-43427	-32227	-32633	-43224	-32430
0,6	0,4	0,179	0,017	0,299	0,042	-26744	-63306	-18790	-49037	-41369	-30889
0,7	0,3	0,392	0,0040	0,560	0,013	-14573	-85860	-9019	-67111	-35959	-26447
0,8	0,2	0,657	0,00085	0,822	0,004	-6518	-109923	-3044	-84861	-27199	-19407
0,9	0,1	0,875	0,00017	0,972	0,001	-2075	-135037	-434	-99181	-15371	-10309
1	0	1	0	1	0	0		0		0	0
1900 K											
0	1	0	1		1		0		0	0	0
0,1	0,9	0,0001	0,874	0,001	0,971	-135661	-2119	-99288	-455	-15474	-10338
0,2	0,8	0,0009	0,655	0,004	0,819	-109887	-6678	-84463	-3153	-27320	-19415
0,3	0,7	0,004	0,389	0,014	0,557	-85380	-14878	-66361	-9244	-36029	-26379
0,4	0,6	0,018	0,179	0,047	0,299	-62666	-27131	-48191	-19061	-41345	-30713
0,5	0,5	0,066	0,064	0,132	0,128	-42858	-43343	-31909	-32394	-43101	-32151
0,6	0,4	0,184	0,018	0,307	0,046	-26716	-63058	-18647	-48583	-41253	-30622
0,7	0,3	0,396	0,004	0,566	0,014	-14619	-85479	-8985	-66460	-35877	-26227
0,8	0,2	0,659	0,0009	0,824	0,004	-6572	-109524	-3047	-84100	-27163	-19258
0,9	0,1	0,875	0,0001	0,972	0,001	-2102	-134804	-438	-98431	-15372	-10237
1	0	1	0	1	0	0		0		0	0
1973 K											
0	1	0	1		1		0		0	0	0
0,1	0,9	0,0002	0,874	0,002	0,971	-135409	-2200	-97638	-471	-15521	-10188
0,2	0,8	0,001	0,657	0,006	0,822	-108968	-6871	-82568	-3211	-27291	-19082
0,3	0,7	0,005	0,397	0,019	0,568	-84305	-15116	-64556	-9265	-35873	-25852

0,4	0,6	0,023	0,190	0,057	0,316	-61823	-27237	-46792	-18858	-41071	-30032
0,5	0,5	0,075	0,072	0,150	0,144	-42418	-43117	-31048	-31747	-42767	-31397
0,6	0,4	0,197	0,022	0,328	0,055	-26640	-62389	-18260	-47358	-40939	-29900
0,7	0,3	0,407	0,005	0,581	0,019	-14742	-84448	-8892	-64698	-35654	-25634
0,8	0,2	0,663	0,001	0,829	0,006	-6718	-108444	-3058	-82044	-27063	-18855
0,9	0,1	0,875	0,0002	0,973	0,002	-2175	-134174	-446	-96403	-15375	-10042
1	0	1	0	1	0	0		0		0	0

Table 3. Thermodynamic properties of Ni-Fe binary system at 1873, 1900 and 1973 K.

X_{Ni}	X_{Fe}	a_{Ni}	a_{Fe}	γ_{Ni}	γ_{Fe}	Gm Ni	Gm Fe	Gxs Ni	Gxs Fe	ΔGm	ΔGxs
1873 K											
0	1	0	1		1		0		0	0	0
0,1	0,9	0,075	0,899	0,750	0,999	-40324	-1645	-4468	-4	-5513	-450
0,2	0,8	0,152	0,797	0,764	0,996	-29255	-3531	-4192	-56	-8675	-883
0,3	0,7	0,236	0,690	0,787	0,986	-22465	-5772	-3717	-218	-10780	-1267
0,4	0,6	0,327	0,579	0,819	0,965	-17372	-8507	-3103	-552	-12053	-1572
0,5	0,5	0,428	0,465	0,856	0,930	-13208	-11915	-2414	-1121	-12561	-1767
0,6	0,4	0,537	0,352	0,896	0,880	-9665	-16255	-1710	-1986	-12301	-1821
0,7	0,3	0,654	0,244	0,934	0,813	-6610	-21959	-1055	-3210	-11214	-1702
0,8	0,2	0,774	0,146	0,967	0,732	-3986	-29917	-511	-4854	-9172	-1379
0,9	0,1	0,892	0,063	0,991	0,638	-1779	-42838	-138	-6982	-5885	-823
1	0	1	0	1	0	0		0		0	0
1900 K											
0	1	0	1		1		0		0	0	0
0,1	0,9	0,075	0,899	0,757	0,999	-40756	-1669	-4383	-5	-5578	-443
0,2	0,8	0,154	0,797	0,771	0,996	-29524	-3582	-4100	-57	-8771	-866
0,3	0,7	0,238	0,690	0,794	0,986	-22646	-5853	-3628	-219	-10891	-1241
0,4	0,6	0,330	0,579	0,825	0,965	-17498	-8617	-3024	-547	-12169	-1538
0,5	0,5	0,430	0,466	0,861	0,932	-13298	-12053	-2349	-1104	-12676	-1726
0,6	0,4	0,540	0,353	0,900	0,884	-9732	-16422	-1663	-1948	-12408	-1777
0,7	0,3	0,656	0,245	0,937	0,819	-6660	-22158	-1025	-3139	-11309	-1659
0,8	0,2	0,775	0,148	0,969	0,740	-4021	-30161	-496	-4738	-9249	-1344
0,9	0,1	0,892	0,065	0,991	0,650	-1799	-43176	-134	-6803	-5936	-801
1	0	1	0	1	0	0		0		0	0
1973 K											
0	1	0	1		1		0		0	0	0
0,1	0,9	0,077	0,899	0,776	0,999	-41922	-1735	-4152	-7	-5754	-422
0,2	0,8	0,158	0,796	0,790	0,996	-30252	-3723	-3852	-63	-9029	-821
0,3	0,7	0,244	0,690	0,813	0,986	-23136	-6072	-3386	-221	-11191	-1170
0,4	0,6	0,337	0,580	0,842	0,967	-17840	-8914	-2809	-535	-12484	-1445
0,5	0,5	0,437	0,468	0,875	0,937	-13544	-12429	-2174	-1058	-12986	-1616
0,6	0,4	0,546	0,357	0,910	0,893	-9914	-16876	-1534	-1845	-12699	-1659
0,7	0,3	0,660	0,250	0,944	0,835	-6794	-22698	-944	-2949	-11565	-1545
0,8	0,2	0,778	0,152	0,972	0,763	-4116	-30823	-455	-4423	-9457	-1249
0,9	0,1	0,893	0,068	0,992	0,680	-1851	-44090	-123	-6320	-6075	-743
1	0	1	0	1	0	0		0		0	0

3. SUMMARY

The liquidus projection and the reaction scheme for the whole concentration range in the investigated binary systems have been constructed, which are of interest for engineering applications, as well as for further basic materials researches.

4. ACKNOWLEDGEMENTS

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