Investigation of thermodynamic Properties Composition of Al-Fe-Ni system

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***Abstract*—** *Thermodynamic properties of the Al-Fe–Ni system and its constituent's binary systems in a wide temperature range of 1873-1973 K and the whole range of concentrations have been studied using the FactSage.*

Keywords*— *Al-Fe-Ni, FactSage, thermodynamic properties.

I. INTRODUCTION

The ternary system Al-Fe-Ni as well as the other aluminides are of interest as high temperature structural materials due to their very high melting temperatures, good oxidation resistance and low mass density. Knowledge of Al-Fe-Ni and its constituent's binary systems, their fundamental physical and chemical properties is the necessary prerequisite for the development of technical alloys [1].

A thorough knowledge of the phase equilibria and thermodynamic properties of the Al–Fe–Ni 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]. In addition to the technological importance, the Al–Fe–Ni system attracts basic scientific interest due to the existence of the decagonal quasi-crystalline phase τ3 and the order/disorder transitions between BCC A2 and BCC B2 phases, as well as between FCC A1 and L12 phases [2].

The Al–Fe–Ni system has been critically assessed by Rivlin and Raynor [3]. According to the recent work by Eleno et al. [4] and Zhang et al. [5,6], the Al–Fe–Ni system is extremely complex due to the existence of plentiful experimental data and 16 stable phases.

Using limited experimental data, Kaufman and Nesor [7] first computed several isothermal sections from 427 to 1607 ^{0}C. Mainly based on their own experimental data and supplemented with the data reported by Bradley and Taylor [8], Jia et al. [9] carried out a thermodynamic calculation for the Al–Fe–Ni system in the Ni-rich region. The phase equilibria computed by Jia et al. [9] agree well with the experimental ones. The work by Dupin et al. [10] and Du et al. [11] indicate that it is possible to describe the thermodynamic properties of disordered and ordered phases using a single equation.

So far no thermodynamic modeling has been performed over the entire temperature and composition ranges for the Al–Fe–Ni system. Because of that, the purposes of the present work are to briefly evaluate the measured thermodynamic data available for the Al–Fe–Ni system and its constituent's binary systems and to obtain an optimal set of thermodynamic parameters for the ternary system over the whole composition and temperature ranges.

II. RESULTS

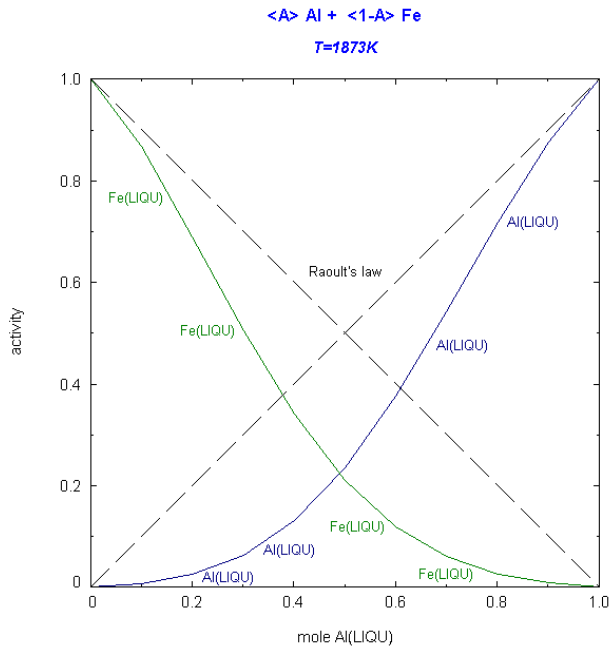
Thermodynamic properties of the Al-Fe–Ni system and its constituent's binary systems in a wide temperature range of 1873-1973 K and the whole range of concentrations have been studied using the FactSage [12].

The thermodynamic calculations in Al-Fe-Ti 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.

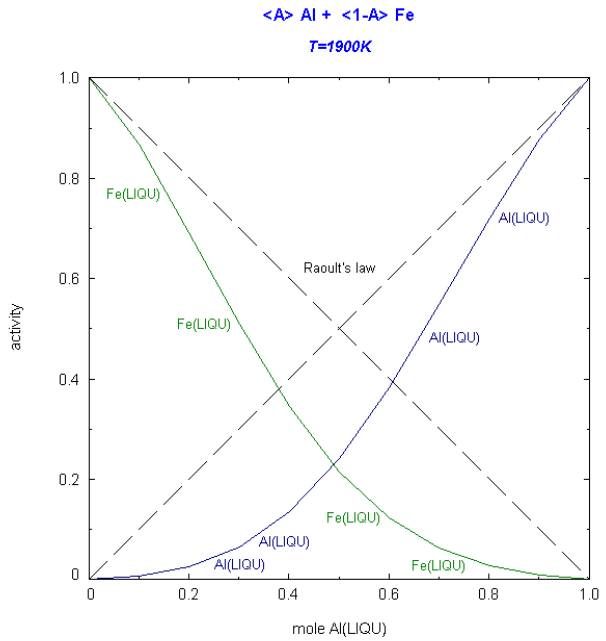
The results of activities for the investigated binary systems are shown in Figs. 1-3, respectively.

TABLE 1
COMPOSITION OF Al-Fe-Ni TERNARY SYSTEMS IN THE INVESTIGATED SECTIONS

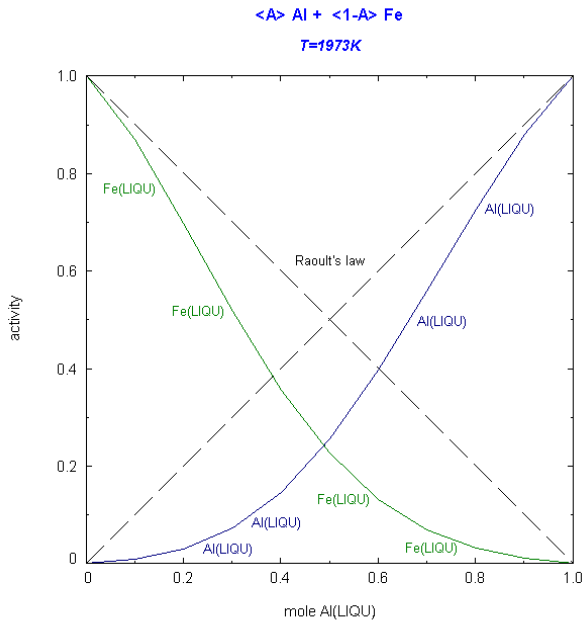
Cross section	A	B	C	D	E
$x_{Al} : x_{Fe}$	9:1	7:3	5:5	3:7	1:9
$x_{Fe} : x_{Ni}$	9:1	7:3	5:5	3:7	1:9
$x_{Ni} : x_{Al}$	9:1	7:3	5:5	3:7	1:9



(a)

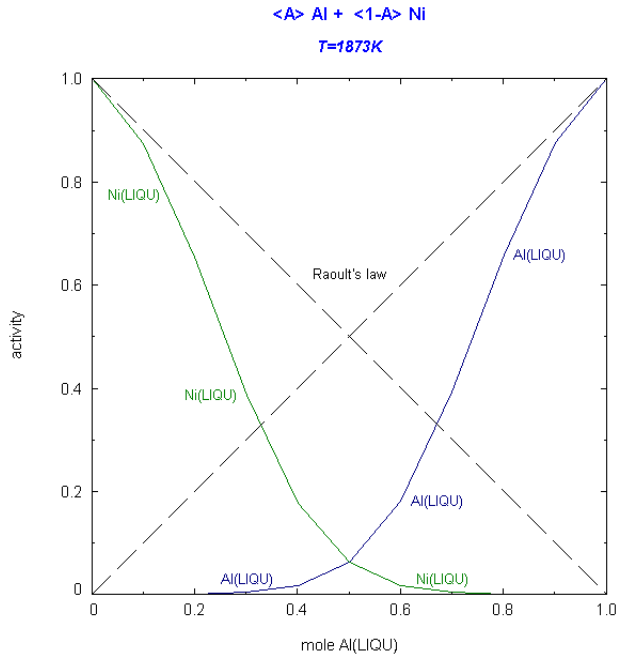


(b)

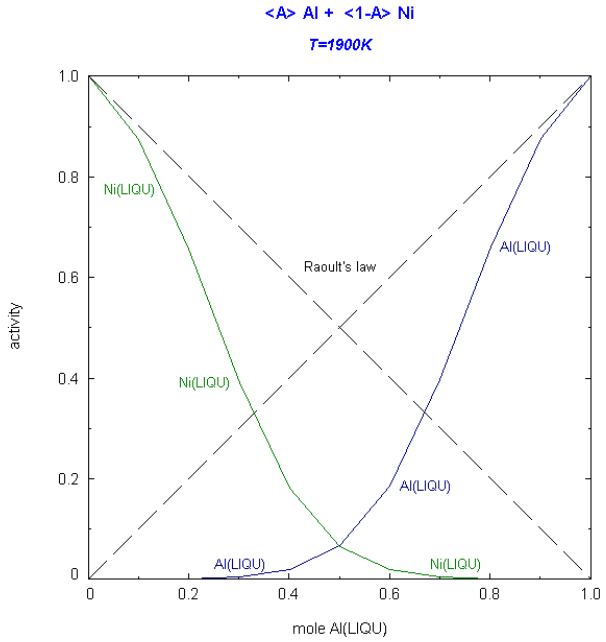


(c)

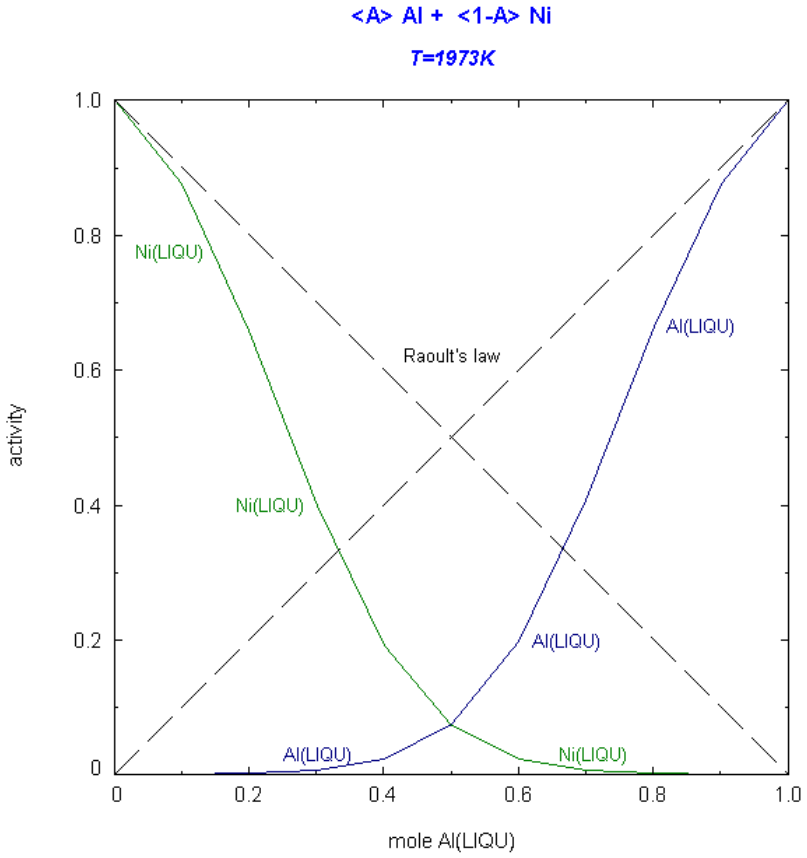
FIGURE 1. ACTIVITY OF Al AND Fe AT a) 1873K, b) 1900K, c) 1973K



(a)

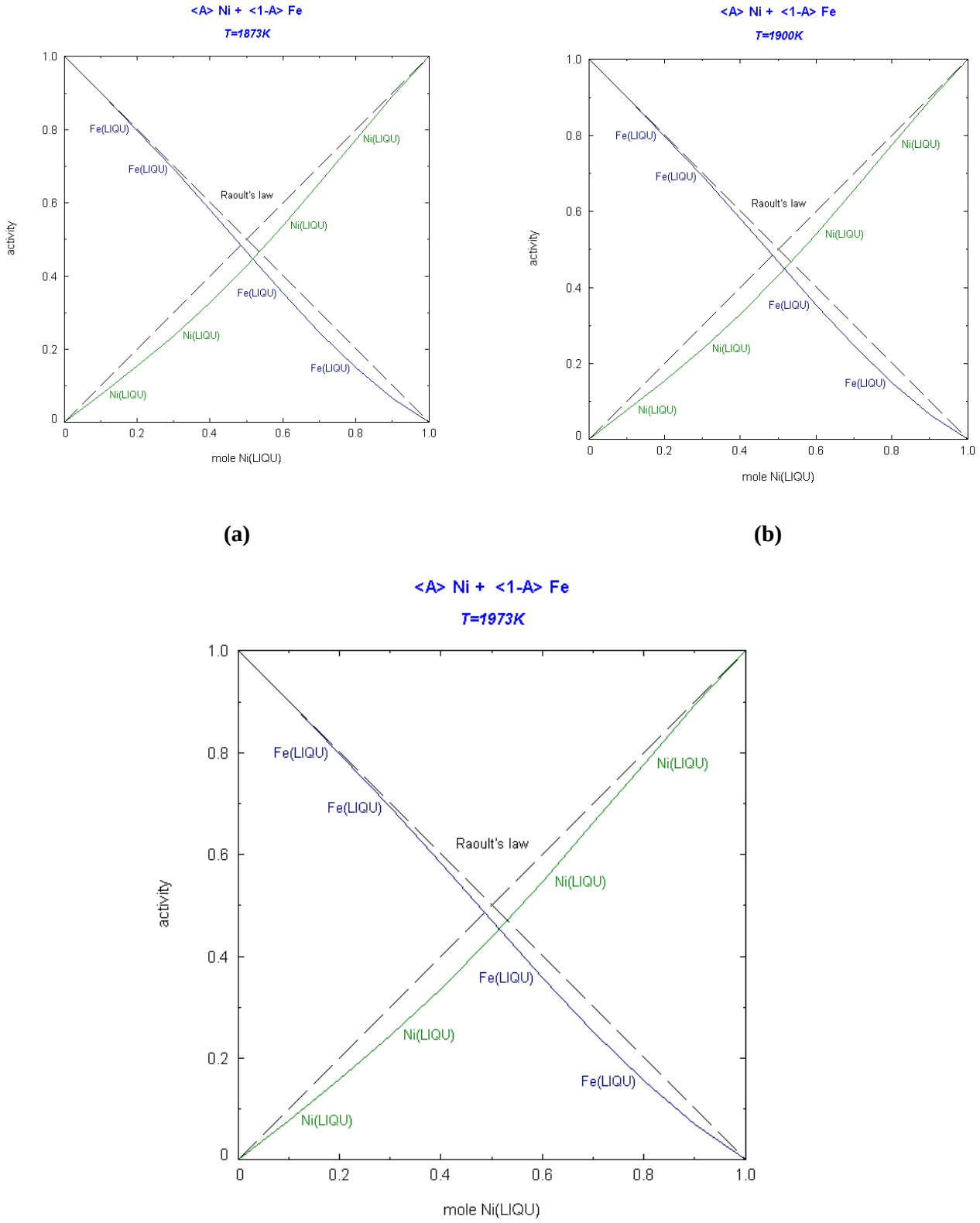


(b)



(c)

FIGURE 2. ACTIVITY OF Al AND Ni AT a) 1873K, b) 1900K, c) 1973K



(a) **(b)**

(c)

FIGURE 1. ACTIVITY OF Ni AND Fe AT a) 1873K, b) 1900K, c) 1973K

Values for the integral Gibbs energy of mixing and integral excess Gibbs energy of Al-Fe-Ni ternary system at 1873K, 2000K and 2073K are presented in Tables 2, 3 and 4.

TABLE 2
INTEGRAL GIBBS ENERGY OF MIXING AND EXCESS GIBBS ENERGY FOR Al-Fe-Ni TERNARY SYSTEM AT 1873K

x_{Al}	x_{Fe}	x_{Ni}	ΔG^M	ΔG^E	x_{Fe}	x_{Ni}	ΔG^M	ΔG^E
Cross section A					**Cross section B**			
0	0,9	0,1	-5885	-823	0,7	0,3	-11214	-1702
0,1	0,81	0,09	-20343	-10725	0,63	0,27	-24170	-10547
0,2	0,72	0,08	-31022	-19180	0,56	0,24	-33140	-17738
0,3	0,63	0,07	-38596	-25540	0,49	0,21	-39113	-22942
0,4	0,54	0,06	-42924	-29407	0,42	0,18	-42146	-25958
0,5	0,45	0,05	-43897	-30572	0,35	0,15	-42242	-26692
0,6	0,36	0,04	-41495	-28990	0,28	0,12	-39432	-25147
0,7	0,27	0,03	-35799	-24767	0,21	0,09	-33794	-21428
0,8	0,18	0,02	-26979	-18174	0,14	0,06	-25439	-15745
0,9	0,09	0,01	-15247	-9679	0,07	0,03	-14449	-8436
1	0	0	0	0	0	0	0	0
Cross section C					**Cross section D**			
0	0,5	0,5	-12561	-1767	0,3	0,7	-10780	-1267
0,1	0,45	0,45	-24265	-9489	0,27	0,63	-21453	-7830
0,2	0,4	0,4	-31977	-15549	0,24	0,56	-28264	-12861
0,3	0,35	0,35	-36876	-19808	0,21	0,49	-32504	-16333
0,4	0,3	0,3	-39145	-22188	0,18	0,42	-34427	-18239
0,5	0,25	0,25	-38861	-22671	0,15	0,35	-34154	-18604
0,6	0,2	0,2	-36088	-21290	0,12	0,28	-31760	-17474
0,7	0,15	0,15	-30888	-18138	0,09	0,21	-27291	-14925
0,8	0,1	0,1	-23321	-13370	0,06	0,14	-20757	-11062
0,9	0,05	0,05	-13359	-7217	0,03	0,07	-12039	-6026
1	0	0	0	0	0	0	0	0
Cross section E								
0	0,1	0,9	-5513	-450				
0,1	0,09	0,81	-15452	-5833				
0,2	0,08	0,72	-21752	-9910				
0,3	0,07	0,63	-25762	-12706				
0,4	0,06	0,54	-27770	-14253				
0,5	0,05	0,45	-27913	-14589				
0,6	0,04	0,36	-26264	-13759				
0,7	0,03	0,27	-22850	-11819				
0,8	0,02	0,18	-17634	-8829				
0,9	0,01	0,09	-10431	-4862				
1	0	0	0	0				

TABLE 3
INTEGRAL GIBBS ENERGY OF MIXING AND EXCESS GIBBS ENERGY FOR Al-Fe-Ni TERNARY SYSTEM AT 1900K

x_{Al}	x_{Fe}	x_{Ni}	ΔG^M	ΔG^E	x_{Fe}	x_{Ni}	ΔG^M	ΔG^E
Cross section A					**Cross section B**			
0	0,9	0,1	-5936	-801	0,7	0,3	-11309	-1659
0,1	0,81	0,09	-20405	-10648	0,63	0,27	-24265	-10445
0,2	0,72	0,08	-31049	-19036	0,56	0,24	-33201	-17576
0,3	0,63	0,07	-38577	-25333	0,49	0,21	-39134	-22730
0,4	0,54	0,06	-42865	-29152	0,42	0,18	-42133	-25712
0,5	0,45	0,05	-43816	-30299	0,35	0,15	-42212	-26438
0,6	0,36	0,04	-41418	-28733	0,28	0,12	-39403	-24912
0,7	0,27	0,03	-35747	-24557	0,21	0,09	-33780	-21236
0,8	0,18	0,02	-26962	-18030	0,14	0,06	-25445	-15610
0,9	0,09	0,01	-15256	-9608	0,07	0,03	-14467	-8367
1	0	0	0	0	0	0	0	0
Cross section C					**Cross section D**			
0	0,5	0,5	-12676	-1726	0,3	0,7	-10891	-1241
0,1	0,45	0,45	-24377	-9388	0,27	0,63	-21566	-7746
0,2	0,4	0,4	-32058	-15394	0,24	0,56	-28353	-12729
0,3	0,35	0,35	-36924	-19610	0,21	0,49	-32568	-16163
0,4	0,3	0,3	-39167	-21966	0,18	0,42	-34470	-18049
0,5	0,25	0,25	-38868	-22444	0,15	0,35	-34183	-18408
0,6	0,2	0,2	-36091	-21080	0,12	0,28	-31781	-17290
0,7	0,15	0,15	-30897	-17963	0,09	0,21	-27311	-14767
0,8	0,1	0,1	-23339	-13244	0,06	0,14	-20778	-10944
0,9	0,05	0,05	-13381	-7150	0,03	0,07	-12061	-5960
1	0	0	0	0	0	0	0	0
Cross section E								
0	0,1	0,9	-5578	-443				
0,1	0,09	0,81	-15532	-5775				
0,2	0,08	0,72	-21823	-9810				
0,3	0,07	0,63	-25818	-12573				
0,4	0,06	0,54	-27811	-14098				
0,5	0,05	0,45	-27941	-14424				
0,6	0,04	0,36	-26284	-13599				
0,7	0,03	0,27	-22866	-11676				
0,8	0,02	0,18	-17650	-8718				
0,9	0,01	0,09	-10447	-4798				
1	0	0	0	0				

TABLE 4
INTEGRAL GIBBS ENERGY OF MIXING AND EXCESS GIBBS ENERGY FOR Al-Fe-Ni TERNARY SYSTEM AT 1973K

x_{Al}	x_{Fe}	x_{Ni}	ΔG^M	ΔG^E	x_{Fe}	x_{Ni}	ΔG^M	ΔG^E
Cross section A					**Cross section B**			
0	0,9	0,1	-6075	-743	0,7	0,3	-11565	-1545
0,1	0,81	0,09	-20570	-10438	0,63	0,27	-24522	-10171
0,2	0,72	0,08	-31124	-18650	0,56	0,24	-33364	-17140
0,3	0,63	0,07	-38526	-24773	0,49	0,21	-39188	-22154
0,4	0,54	0,06	-42702	-28463	0,42	0,18	-42099	-25047
0,5	0,45	0,05	-43596	-29560	0,35	0,15	-42132	-25751
0,6	0,36	0,04	-41210	-28037	0,28	0,12	-39325	-24277
0,7	0,27	0,03	-35607	-23987	0,21	0,09	-33741	-20714
0,8	0,18	0,02	-26916	-17641	0,14	0,06	-25458	-15246
0,9	0,09	0,01	-15282	-9416	0,07	0,03	-14515	-8180
1	0	0	0	0	0	0	0	0
Cross section C					**Cross section D**			
0	0,5	0,5	-12986	-1616	0,3	0,7	-11191	-1170
0,1	0,45	0,45	-24680	-9114	0,27	0,63	-21870	-7519
0,2	0,4	0,4	-32277	-14972	0,24	0,56	-28595	-12370
0,3	0,35	0,35	-37054	-19074	0,21	0,49	-32741	-15707
0,4	0,3	0,3	-39225	-21364	0,18	0,42	-34586	-17534
0,5	0,25	0,25	-38886	-21831	0,15	0,35	-34260	-17880
0,6	0,2	0,2	-36100	-20512	0,12	0,28	-31838	-16791
0,7	0,15	0,15	-30921	-17490	0,09	0,21	-27365	-14338
0,8	0,1	0,1	-23386	-12903	0,06	0,14	-20836	-10624
0,9	0,05	0,05	-13439	-6969	0,03	0,07	-12118	-5784
1	0	0	0	0	0	0	0	0
Cross section E								
0	0,1	0,9	-5754	-422				
0,1	0,09	0,81	-15751	-5619				
0,2	0,08	0,72	-22014	-9540				
0,3	0,07	0,63	-25967	-12214				
0,4	0,06	0,54	-27919	-13680				
0,5	0,05	0,45	-28017	-13980				
0,6	0,04	0,36	-26337	-13164				
0,7	0,03	0,27	-22908	-11288				
0,8	0,02	0,18	-17692	-8417				
0,9	0,01	0,09	-10491	-4626				
1	0	0	0	0				

III. CONCLUSION

The thermodynamic properties of the investigated Al-Fe-Ni ternary system and its constituent's binary systems at 1873K, 1900K and 1973K were determined. Investigated systems have negative values for integral excess Gibbs energy. Activity values of the components are less than unity and show negative deviation from the Raoult's law.

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

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