

## **THERMODYNAMIC PREDICTING OF Si-Me (Me = Ti, Al) BINARY SYSTEMS**

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### **Abstract**

*Thermodynamic predicting analysis of Si-based binary systems - Ti-Si, and Al-Si, are shown in this paper. Thermodynamic analysis 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: 2000K, 2400K and 2473K, as well as calculation of phase diagrams for the investigated binaries. The FactSage was used for all thermodynamic calculations.*

*Keywords:* Ti-Si, Al-Si, binary systems, thermodynamic predicting, FactSage

### **1. Introduction**

Titanium-based alloys are potentially useful materials for application in the aerospace industry, due to their high oxidation resistance, low density and

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high melting point [1]. Silicon is an important alloying additive to titanium alloys and contributes useful dispersion strengthening and improves microstructure stability.

Some of Ti-based systems were studied thermodynamically using FactSage [2-5], while in the studies of Gros, Ansara and Allibert [6], and Lee, Soh, Lee and Kim [7], CALPHAD methods have been used in phase equilibria predicting of Ti-alloys.

Iwata, Matsumiya, Sawada and Kawakami [8] predicted thermodynamic properties, including activity coefficients and the interaction parameters of the solute elements in infinite dilute Si solutions, by the use of first-principles calculations based on density functional theory.

Palacio and Arranz [9] analyzed the formation of the Si/Ti interface during the deposition of silicon on titanium polycrystalline substrates, which has been studied at room temperature using X-ray photoelectron spectroscopy, angle-resolved XPS, ultraviolet photoelectron spectroscopy and ion scattering spectroscopy.

Bulanova, Tretyachenko, Golovkova and Meleshevich [10] studied phase equilibria in the alpha-Ti-Al-Si region of the ternary Ti-Al-Si system using differential thermal analysis, X-ray diffraction, metallography and microprobe analysis.

The microstructure and electrical properties of the contacts, formed in the Ti-Al-Si system due to rapid thermal processing at temperatures between 300 and 800 °C, were studied extensively by Komem and Katz [11].

Nevertheless, thermodynamic study of the Ti-Al-Si system has not been completely reported in literature. The main reasons are experimental difficulties, especially the high investigation temperatures required. Having a mind such problems, it is anticipated that most of the thermodynamic data of ternary and multi-component systems will come from theoretical calculations rather than from direct experimentation. Therefore, thermodynamic study of liquid Ti-Si and Al-Si binary systems is presented in this paper.

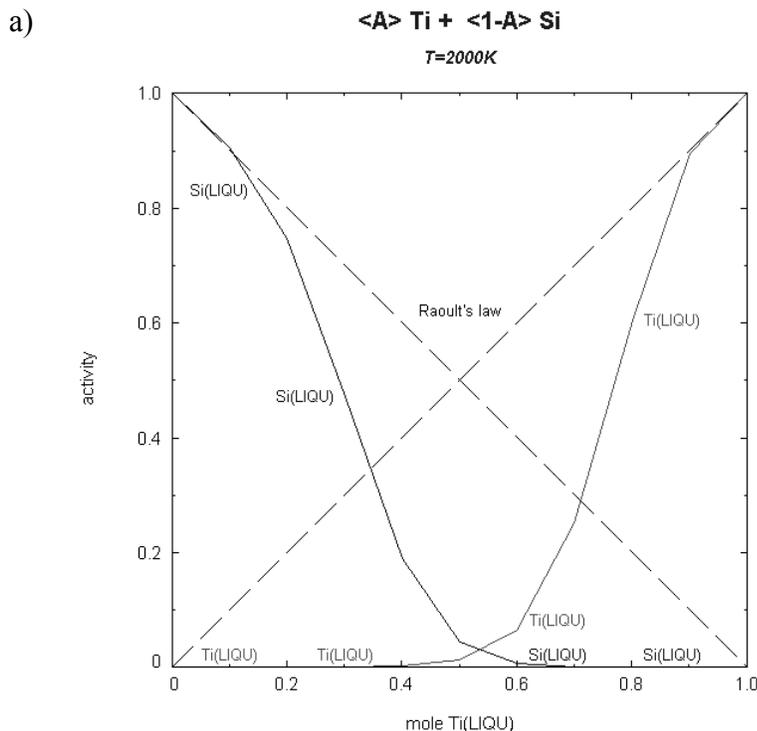
## 2. Results and discussion

The results of thermodynamic analysis and predicting in binaries Ti-Si and Al-Si were obtained using FactSage [12] thermo-chemical software and

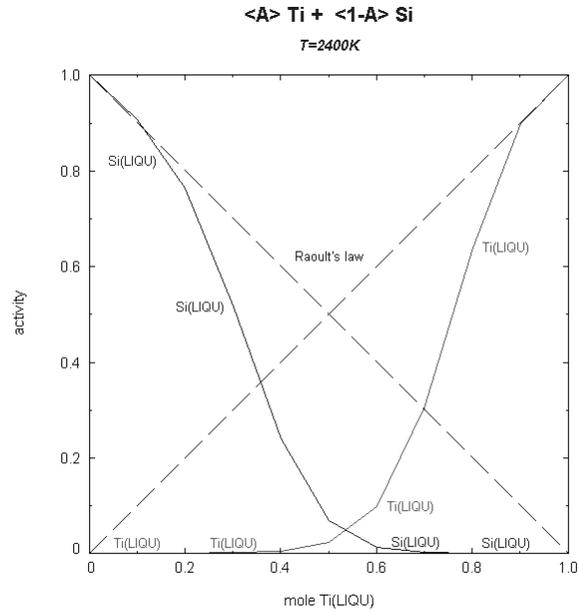
databases. FactSage was introduced in 2001 and it presents the fusion of the FACT-Win/F\*A\*C\*T and ChemSage/SOLGASMIX thermo-chemical packages that were founded over 25 years ago.

Activities of the components in the investigated binaries at three different temperatures - 2000K, 2400K and 2473K, are shown in Figs. 1 and 2, respectively. Partial and integral Gibbs energies of mixing and excess energies for the each investigated binary systems at three different temperatures are given in Tables 1 and 2.

Strong negative deviation from ideal behaviour can be noticed for liquid Ti-Si binary alloys, while relatively negative deviation is typical for Al-Si liquid alloys. Considering calculated integral thermodynamic properties, all constitutive binary systems show negative values for integral Gibbs energy of mixing and integral excess Gibbs energy. There are no thermodynamic data on activities of the components in both binary systems Ti-Si and Al-Si at investigated temperatures, so there is no possibility for comparison between experimental and calculated data.



b)



c)

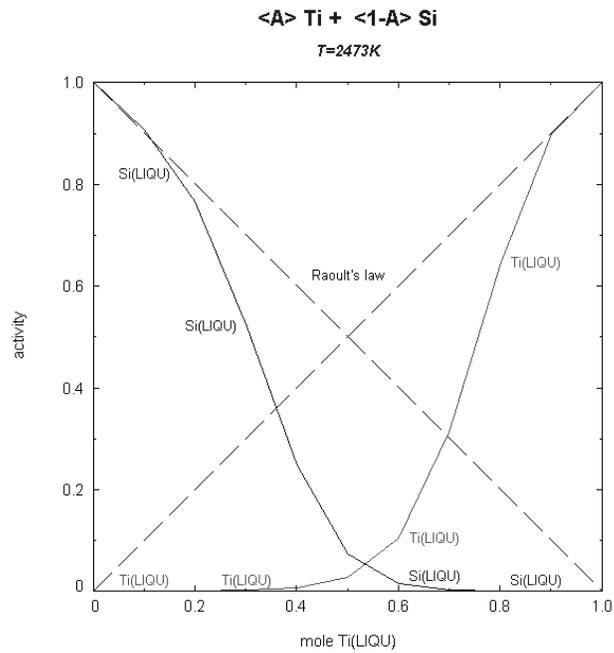


Fig.1. Activity of titanium and silicon in Ti-Si system at a) 2000K, b) 2400K, c) 2473K

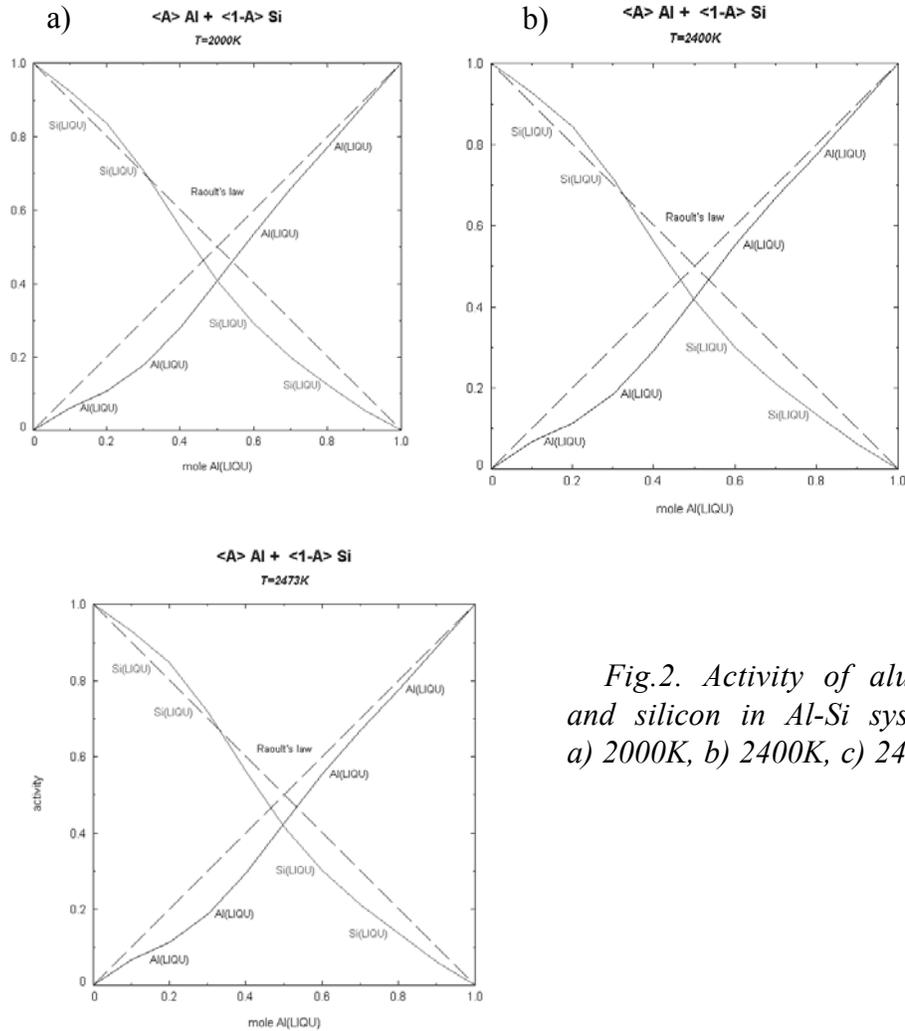


Fig.2. Activity of aluminum and silicon in Al-Si system at a) 2000K, b) 2400K, c) 2473K

Phase diagrams of the investigated binary systems Ti-Si and Al-Si obtained using FactSage thermodynamic software and database are shown in Figs. 3 and 4, respectively.

Table 1. Thermodynamic properties in Ti-Si binary system at 2000K, 2400K and 2473K

T K	$x_{Ti}$	$x_{Si}$	$G_{Ti}^M$ J/mol	$G_{Si}^M$ J/mol	$\Delta G^M$ J/mol	$G_{Ti}^{XS}$ J/mol	$G_{Si}^{XS}$ J/mol	$\Delta G^{XS}$ J/mol
2000	0	1		0	0		0	0
	0,1	0,9	-172136	-1657	-18705	-133849	95	-13299
	0,2	0,8	-154285	-4857	-34743	-127523	-1147	-26422
	0,3	0,7	-131614	-12548	-48268	-111595	-6618	-38111
	0,4	0,6	-103742	-27720	-58129	-88506	-19226	-46938
	0,5	0,5	-73702	-52455	-63078	-62177	-40929	-51553
	0,6	0,4	-45527	-86989	-62111	-37033	-71753	-50921
	0,7	0,3	-22962	-128846	-54727	-17031	-108826	-44569
	0,8	0,2	-8397	-172167	-41151	-4687	-145406	-32831
	0,9	0,1	-1856	-208190	-22490	-104	-169902	-17084
	1	0	0	0	0	0	0	
2400	0	1		0	0		0	0
	0,1	0,9	-175745	-1957	-19336	-129801	145	-12849
	0,2	0,8	-156439	-5399	-35607	-124325	-947	-25622
	0,3	0,7	-133170	-13285	-49250	-109146	-6168	-37061
	0,4	0,6	-104990	-28619	-59168	-86707	-18426	-45739
	0,5	0,5	-74758	-53510	-64134	-60927	-39679	-50303
	0,6	0,4	-46426	-88236	-63150	-36233	-69952	-49721
	0,7	0,3	-23698	-130400	-55708	-16581	-106377	-43519
	0,8	0,2	-8939	-174321	-42016	-4487	-142207	-32031
	0,9	0,1	-2157	-211799	-23121	-54	-165854	-16634
	1	0	0	0	0	0	0	
2473	0	1		0	0		0	0
	0,1	0,9	-176404	-2012	-19451	-129061	154	-12767
	0,2	0,8	-156832	-5498	-35765	-123741	-910	-25476
	0,3	0,7	-133452	-13419	-49429	-108698	-6086	-36869
	0,4	0,6	-105218	-28783	-59357	-86378	-18280	-45520
	0,5	0,5	-74951	-53703	-64327	-60700	-39451	-50075
	0,6	0,4	-46590	-88465	-63340	-36087	-69625	-49502
	0,7	0,3	-23832	-130684	-55888	-16499	-105930	-43328
	0,8	0,2	-9038	-174714	-42174	-4450	-141623	-31885
	0,9	0,1	-2212	-212458	-23236	-45	-165115	-16552
	1	0	0	0	0	0	0	

Table 2. Thermodynamic properties in Al-Si binary system at 2000K, 2400K and 2473K

T K	$x_{Al}$	$x_{Si}$	$G_{Al}^M$ J/mol	$G_{Si}^M$ J/mol	$\Delta G^M$ J/mol	$G_{Al}^{XS}$ J/mol	$G_{Si}^{XS}$ J/mol	$\Delta G^{XS}$ J/mol
2000	0	1		0	0		0	0
	0,1	0,9	-46748	-1314	-5857	-8460	438	-452
	0,2	0,8	-37238	-2978	-9830	-10476	732	-1509
	0,3	0,7	-28755	-5814	-12696	-8736	117	-2539
	0,4	0,6	-21158	-9904	-14405	-5922	-1410	-3215
	0,5	0,5	-14989	-14938	-14964	-3464	-3412	-3438
	0,6	0,4	-10361	-20578	-14448	-1867	-5341	-3257
	0,7	0,3	-6967	-26879	-12941	-1036	-6859	-2783
	0,8	0,2	-4311	-34926	-10434	-601	-8164	-2113
	0,9	0,1	-1990	-48601	-6651	-238	-10314	-1246
	1	0	0	0	0		0	0
2400	0	1		0	0		0	0
	0,1	0,9	-54349	-1485	-6771	-8404	617	-285
	0,2	0,8	-43648	-3365	-11422	-11534	1087	-1437
	0,3	0,7	-33618	-6723	-14792	-9595	394	-2603
	0,4	0,6	-24522	-11619	-16781	-6239	-1426	-3351
	0,5	0,5	-17220	-17576	-17398	-3389	-3745	-3567
	0,6	0,4	-11878	-24077	-16758	-1686	-5794	-3329
	0,7	0,3	-8067	-31150	-14992	-950	-7126	-2803
	0,8	0,2	-5088	-40182	-12107	-636	-8068	-2122
	0,9	0,1	-2391	-56122	-7764	-289	-10177	-1277
	1	0	0	0	0		0	0
2473	0	1		0	0		0	0
	0,1	0,9	-55736	-1516	-6938	-8394	650	-254
	0,2	0,8	-44819	-3436	-11712	-11728	1152	-1424
	0,3	0,7	-34506	-6889	-15174	-9752	445	-2614
	0,4	0,6	-25137	-11932	-17214	-6297	-1429	-3376
	0,5	0,5	-17626	-18057	-17842	-3375	-3805	-3590
	0,6	0,4	-12155	-24716	-17179	-1652	-5876	-3342
	0,7	0,3	-8267	-31928	-15366	-934	-7174	-2806
	0,8	0,2	-5230	-41141	-12412	-642	-8050	-2124
	0,9	0,1	-2464	-57494	-7967	-298	-10151	-1283
	1	0	0	0	0		0	0

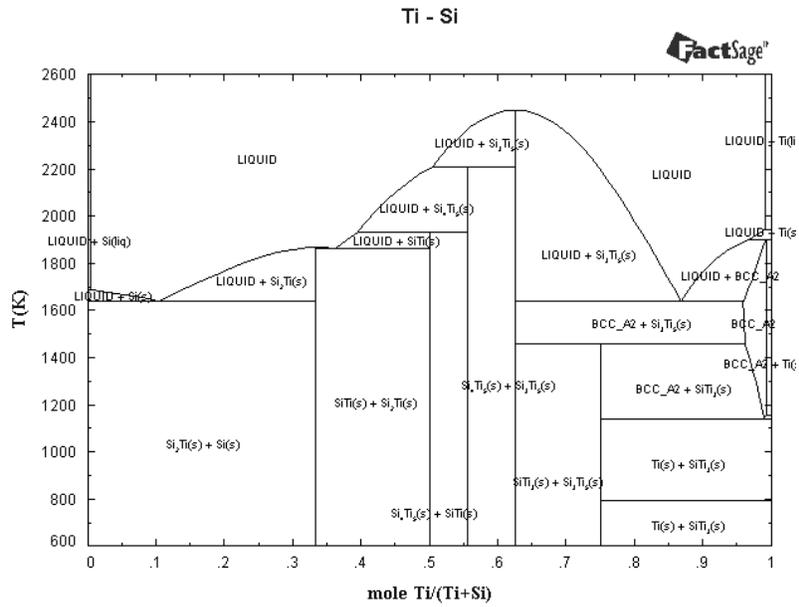


Fig.3. Phase diagram of Ti-Si system

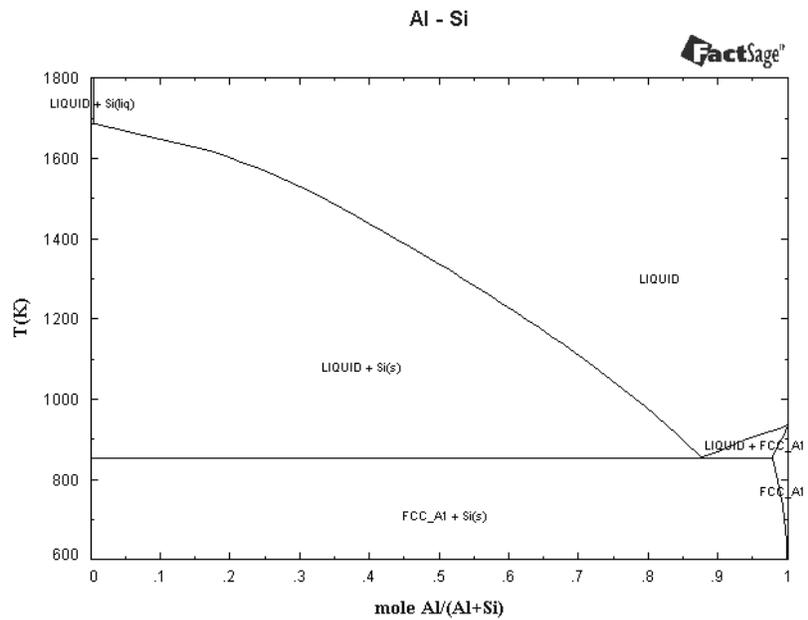


Fig.4. Phase diagram of Al-Si system

There is a good agreement between calculated Ti-Si and Al-Si phase diagrams and literature data from Refs. [13,14] and [15], respectively.

### 3. Conclusions

The thermodynamic properties of binary systems Ti-Si and Al-Si at 2000K, 2400K and 2473K were calculated using the FactSage thermo-chemical software and databases. Investigated binary systems have negative values for integral excess Gibbs energy and the activity values of the components show negative deviation from the Raoult's law.

Providing in mind that no experimental data for Ti-Al-Si-based system have been done or reported, obtained results presented one good base for the further thermodynamic analysis in these ternary system and multi-component systems based on the investigated binaries. Obtained thermodynamic data may be useful as a comparison with some future critical experimental results and for the further thermodynamic optimization of this system.

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