Predicting Thermodynamic Activities in Ti-Al Binary System

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Abstract

In this paper results of predicting thermodynamic calculations in Ti-Al binary system were shown. The activity of Ti and Al as a function of titanium concentration was calculated in the temperature range between 1673 K and 2273 K. Some predicting thermodynamic results were compared to available experimental results. A good agreement has been noticed.

Keywords: *Predicting, Activity, Thermodynamic, Ti-Al binary system*

1. Introduction

Titanium belongs to the fourth group of the periodic table and is comparatively strong and ductile transition metals. Theoretically, the attractive mechanical properties, including the lightweight, strength to weight ratio, high ductility, and low thermal conductivity, result in more functional and comfortable use [1]. Titanium can be alloyed with various elements to change its characteristics, primarily to improve the mechanical property, such as strength, high temperature performance, creep resistance, weldability, response to ageing heat treatments, and formability [2]. Aluminum, a typical alpha stabilizer, increases the alpha-beta transition temperature and maintains the improved mechanical properties over pure titanium.

According to many and extensive application and used especially titanium-aluminum alloys in various fields, it is necessary to know thermodynamic behavior of this binary system as the base binary system for the other alloys based on Ti-Al system.

Many scientists worked on this binary system and there were various interesting and differencing data and results. In the aim of contributing with some more data and approaches of thermodynamic description and determination of this investigated binaries, in this work the results of thermodynamic calculations in Ti-Al are presented. The activity of titanium and aluminum in Ti-Al in the temperature range between 1673 K and 2273K are estimated. Some of the predicting thermodynamic results are compared to available experimental results. A good agreement has been noticed.

2. Results and discussion

The activity of titanium and aluminum in titanium-aluminum alloy is done by the used of FactSage thermochemical databases [3]. The activity of Ti and Al as a function of titanium concentration is calculated in the temperature range between 1673 K and 2273 K. The results are shown in Table 1.

Table 1. Activity Ti and Al in the temperature range from 1673K to 2273K

X_{Ti}	1673K		1773K		1873K		1973K	
	a_{Ti}	a_{Al}	a_{Ti}	a_{Al}	a_{Ti}	a_{Al}	a_{Ti}	a_{Al}
0	0	1	0	1	0	1	0	1
0,1	0,010652	0,90928	0,015141	0,91191	0,020727	0,91426	0,027485	0,91637
0,2	0,024089	0,78796	0,032151	0,79919	0,041609	0,80936	0,052459	0,81860
0,3	0,051639	0,61020	0,064489	0,63285	0,078649	0,65378	0,094007	0,67319
0,4	0,10883	0,40783	0,12757	0,43767	0,14703	0,46617	0,16703	0,49335
0,5	0,21468	0,23373	0,23813	0,26243	0,26123	0,29103	0,28389	0,31938
0,6	0,37792	0,11713	0,40118	0,13875	0,42316	0,16141	0,44393	0,18492
0,7	0,57750	0,053389	0,59423	0,066993	0,60958	0,082052	0,62371	0,098450
0,8	0,76473	0,023063	0,77232	0,030590	0,77915	0,039369	0,78535	0,049389
0,9	0,90128	0,0090298	0,90274	0,012534	0,90404	0,016800	0,90521	0,021859
1	1	0	1	0	1	0	1	0

X_{Ti}	2073K		2173K		2273K	
	a_{Ti}	a_{Al}	a_{Ti}	a_{Al}	a_{Ti}	a_{Al}
0	0	1	0	1	0	1
0,1	0,035467	0,91829	0,044707	0,92003	0,055217	0,92163
0,2	0,064677	0,82705	0,078218	0,83479	0,093026	0,84191
0,3	0,11045	0,69121	0,12785	0,70800	0,14610	0,72366
0,4	0,18743	0,51928	0,20810	0,54400	0,22893	0,56756
0,5	0,30605	0,34737	0,32767	0,37489	0,34872	0,40190
0,6	0,46358	0,20910	0,48218	0,23377	0,49978	0,25880
0,7	0,63676	0,11607	0,64885	0,13478	0,66007	0,15446
0,8	0,79099	0,060617	0,79615	0,073008	0,80088	0,086505
0,9	0,90627	0,027728	0,90724	0,034412	0,90812	0,041902
1	1	0	1	0	1	0

Based on the activity data in Table 1, the activity relationships were calculated for Ti and Al in dependence of Ti composition in the temperatures 1673K - 2273K as follows:

- for titanium

$$a_{Ti} = 0{,}0327 - 0{,}8261x_{Ti} + 3{,}2786x_{Ti}^2 - 1{,}4569x_{Ti}^3 \quad \text{for T=1673K} \ldots\ldots\ldots (1)$$

$$a_{Ti} = 0{,}0308 - 0{,}7503x_{Ti} + 3{,}225x_{Ti}^2 - 1{,}4809x_{Ti}^3 \quad \text{for T=1773K} \ldots\ldots\ldots (2)$$

$$a_{Ti} = 0{,}0290 - 0{,}6617x_{Ti} + 3{,}1308x_{Ti}^2 - 1{,}4769x_{Ti}^3 \quad \text{for T=1873K} \ldots\ldots\ldots (3)$$

$$a_{Ti} = 0{,}0274 - 0{,}5619x_{Ti} + 2{,}9999x_{Ti}^2 - 1{,}4471x_{Ti}^3 \quad \text{for T=1973K} \ldots\ldots\ldots (4)$$
$$a_{Ti} = 0{,}0261 - 0{,}4521x_{Ti} + 2{,}8356x_{Ti}^2 - 1{,}3937x_{Ti}^3 \quad \text{for T=2073K} \ldots\ldots\ldots (5)$$
$$a_{Ti} = 0{,}0252 - 0{,}3337x_{Ti} + 2{,}6413x_{Ti}^2 - 1{,}3189x_{Ti}^3 \quad \text{for T=2173K} \ldots\ldots\ldots (6)$$
$$a_{Ti} = 0{,}0246 - 0{,}2077x_{Ti} + 2{,}4198x_{Ti}^2 - 1{,}2244x_{Ti}^3 \quad \text{for T=2273K} \ldots\ldots\ldots (7)$$

- for aluminum

$$a_{Al} = 1{,}0242 - 1{,}1152x_{Ti} - 1{,}6444x_{Ti}^2 + 1{,}7688x_{Ti}^3 \quad \text{for T=1673K} \ldots\ldots\ldots (8)$$
$$a_{Al} = 1{,}0191 - 0{,}9633x_{Ti} - 1{,}8714x_{Ti}^2 + 1{,}8464x_{Ti}^3 \quad \text{for T=1773K} \ldots\ldots\ldots (9)$$
$$a_{Al} = 1{,}0145 - 0{,}8286x_{Ti} - 2{,}0499x_{Ti}^2 + 1{,}8922x_{Ti}^3 \quad \text{for T=1873K} \ldots\ldots\ldots (10)$$
$$a_{Al} = 1{,}0103 - 0{,}7102x_{Ti} - 2{,}1834x_{Ti}^2 + 1{,}9088x_{Ti}^3 \quad \text{for T=1973K} \ldots\ldots\ldots (11)$$
$$a_{Al} = 1{,}0065 - 0{,}6069x_{Ti} - 2{,}2755x_{Ti}^2 + 1{,}8989x_{Ti}^3 \quad \text{for T=2073K} \ldots\ldots\ldots (12)$$
$$a_{Al} = 1{,}0030 - 0{,}5178x_{Ti} - 2{,}3295x_{Ti}^2 + 1{,}8648x_{Ti}^3 \quad \text{for T=2173K} \ldots\ldots\ldots (13)$$
$$a_{Al} = 1{,}0000 - 0{,}4420x_{Ti} - 2{,}3486x_{Ti}^2 + 1{,}8088x_{Ti}^3 \quad \text{for T=2273K} \ldots\ldots\ldots (14)$$

The dependences Ti and Al activity of Ti content are shown in Fig.1 and Fig.2 respectively.

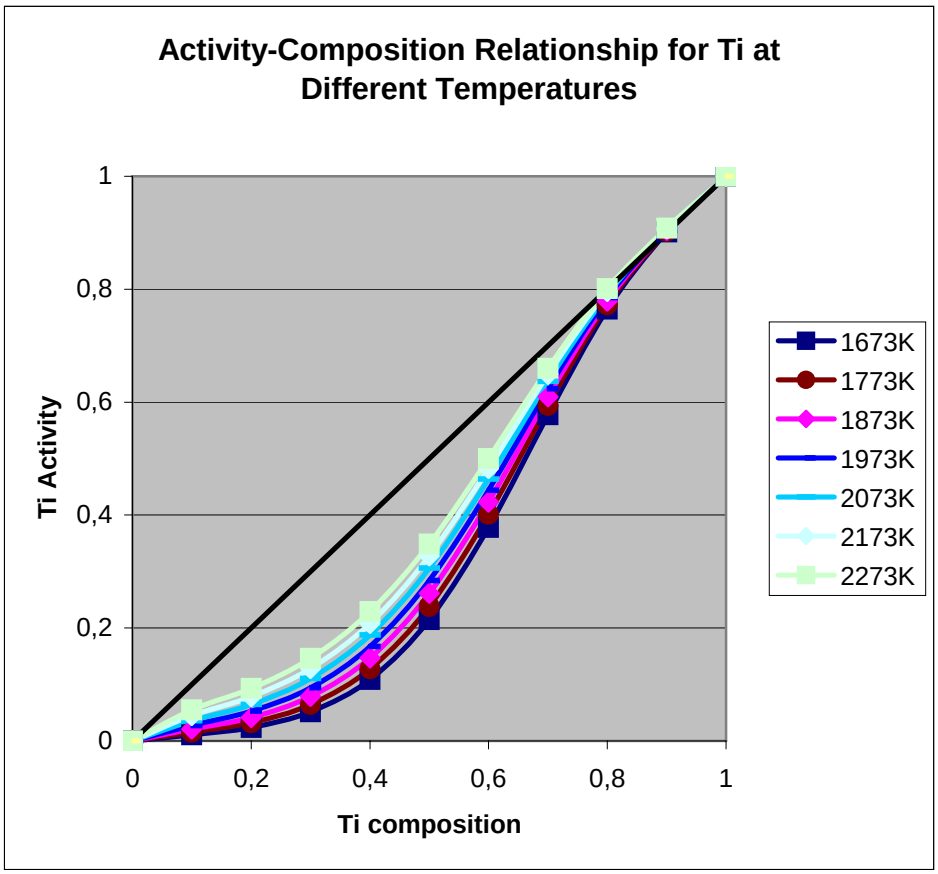

Fig.1. Dependence Ti activity of Ti content in temperature range 1673K-2273K

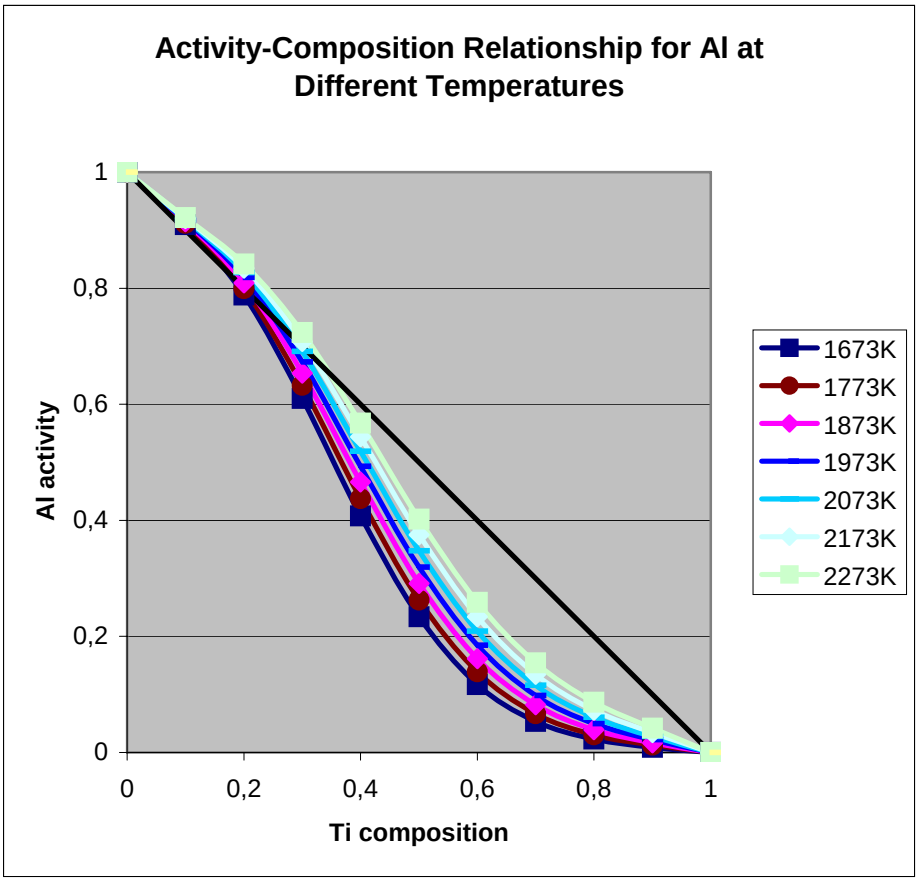

Fig.2. Dependence Al activity of Ti content in the temperature range 1673K-2273K

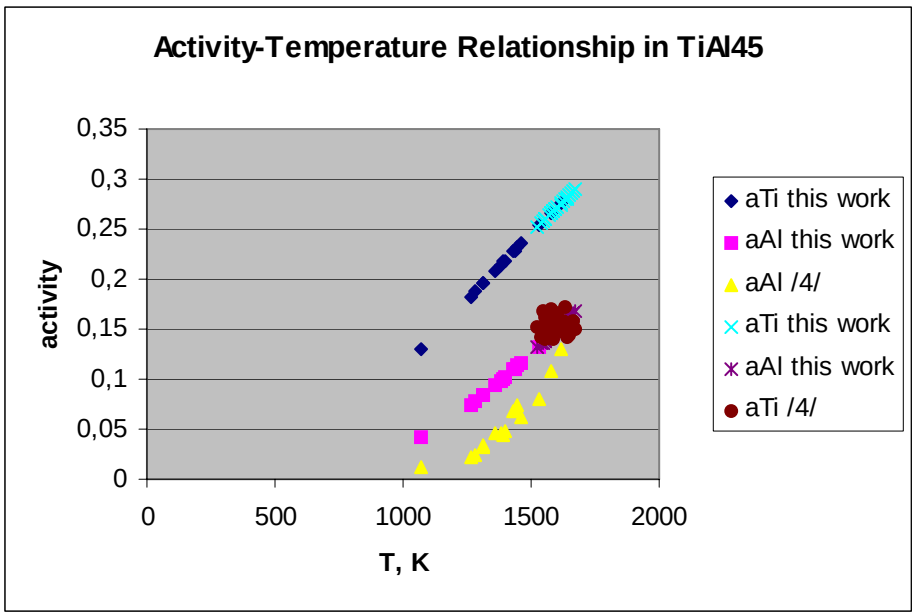

Fig.3. Comparing between experimentally obtained and calculated values for titanium and aluminum activity in TiAl45 alloy at different temperature

Table 1 as well as Fig.1 and Fig.2 show that the activity coefficients of both components are less than unity and activity of both titanium and aluminum increase with the temperature increasing. There is negative deviation of Raoult's law and because of that good miscibility between the components.

Calculating activity of titanium and aluminum from this work are graphically compared with literature results [4] in Fig. 3 and Fig. 4, respectively.

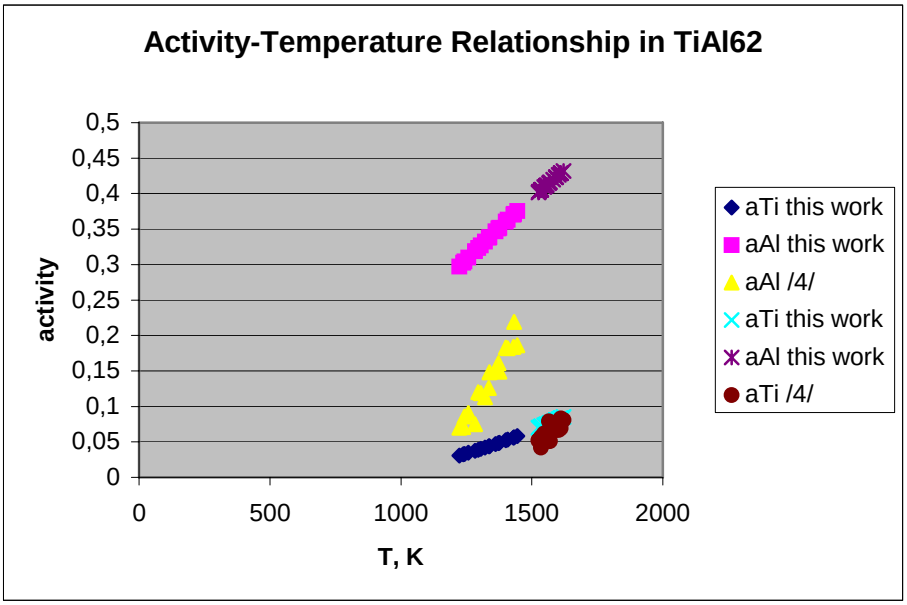

Fig.4. Comparing between experimentally obtained and calculated values for titanium and aluminum activity in TiAl62 alloy at different temperature

Results presented in those Figures show good agreement between calculated and literature results for two different alloys TiAl45 and TiAl62. Good agreement can be noticed especially for titanium activity. Also good agreement is better on higher temperatures.

3. Conclusions

The activity of titanium and aluminum in Ti-Al alloys was calculated at temperature 1673K – 2273K. The activity coefficients of both components are less than unity in the whole concentration range. The negative deviation of Raoult's law and good miscibility between the components were noticed. The activity of both components increases with increasing titanium concentration and with temperature increasing.

Comparing of the obtained and calculated results with literature data and experimentally obtained are done in Ti-Al45 and Ti-Al62 alloys. Comparing shows good agreement for the titanium activity especially at higher temperature and slight disagreement with aluminum activity.

Results presented in this paper are contribution to the more complete thermodynamic description of Ti-Al binary system and may be useful for the further thermodynamic assessment of this system and in particular for ternary and multi component systems based of this binary.

References:

1. E.W.Collings, *The Physical Metallurgy of Titanium Alloys*, Metal Park, OH, 1984, The Am. Soc. Metals 3 – 5.
2. M.J.Donachie, Jr., *Titanium and Its Alloys* In: Titanium and Titanium Alloys Source Book, M.J. Donachie Jr (ed.), Ohio, 1982, Am. Soc. Metals 10 – 19.
3. C.W.Bale, P.Chartrand, S.A.Degterov, G.Eriksson, K.Hack, R.B.Mahfoud, J.Melancon, A.D.Pelton and S.Petersen, *Calphad*, 2002, Vol.26, No.2, p.189.
4. N.S.Jacobson, M.P.Brady and G.M.Mehrotra, *Oxidation of Metals*, 1999, Vol.52, No.516, p.537.

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