Thermodynamic study of Ti–V and Al–V systems using FactSage

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THERMODYNAMIC STUDY OF Ti-V AND Al-V SYSTEMS USING FACTSAGE

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Abstract

Thermodynamic study of Ti-V and Al-V binary systems is presented in this paper. Investigations included thermodynamic determination of activities, coefficient of activities, partial and integral values Gibbs energies of mixing and excess energies at four different temperatures: 2000K, 2073K, 2200K and 2273K, as well as calculated phase diagrams for the investigated systems. The FactSage program was used for all thermodynamic calculations.

Keywords: thermodynamics, Ti-V, Al-V, calculation of phase diagrams, FactSage

1. Introduction

Due to the combination of low weight and high strength, titanium-based and some aluminum-based 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 aluminum are brittle and provide

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moderate resistance to oxidation, alloying with vanadium enhances their ductility, strength, oxidation, and corrosion resistance.

Thermodynamic study of such high temperature systems, for example Al-V and Ti-V systems, has not been completely reported in literature. It is anticipated that most of their thermodynamic data will come from theoretical calculations, rather than from direct experimentation. The main reasons are experimental difficulties, especially high investigation temperatures required.

In the frame of thermodynamic investigations of the Al-V system, enthalpies of formation of solid Al-V alloys have been determined by Kubaschewski et al. [1], as well as by Neckel et al. [2] using high-temperature reaction calorimetry. Results obtained by Neckel et al. [2], which are in fairly good agreement with those published by Kubaschewski et al. [1], are compiled for 298 K and presented in Hultgren book [3]. There are data on thermodynamic activities of the components obtained for solid alloys at 1273K by Johnson et al. [4], using isopiestic method.

Considering the phase diagram of Al-V system, Hansen et al. [5] and Elliott [6] have constructed a phase diagram. The phase equilibria in Al-V system has been studied by Willey [7] and the diagram is assessed by Murray [8]. The Al-V phase diagram, according to [7,8] is presented in Fig. 1.

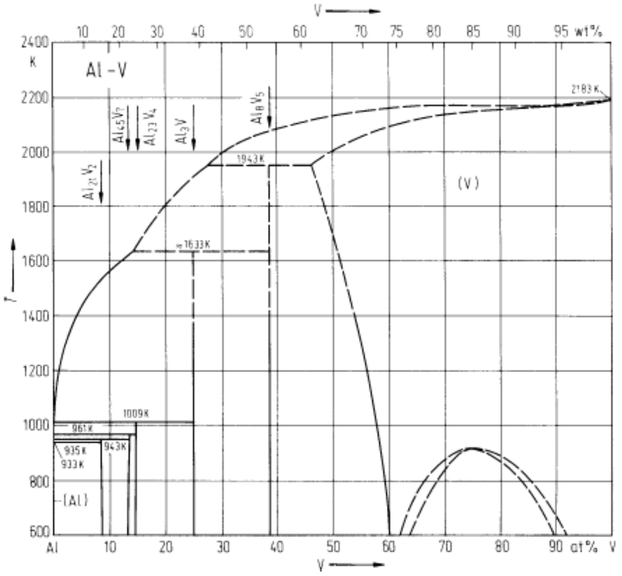

Fig.1. Phase diagram of Al-V system

The other system of interest, Ti-V system, has not yet been investigated thermodynamically. Even an experimentally determined phase diagram is not known, although there were efforts in that topic. So, Miedema et al. [9], applying their model, stated that the enthalpy of formation of Tl-V alloys should be positive. Mostly on this basis Smith et al. [10] have calculated a phase diagram, presented in Fig. 2.

Having in mind the lack of thermodynamic data in these two systems, comparative thermodynamic study of chosen alloys in binary systems Ti-V and Al-V has been done using FactSage program and presented in this paper. The similar calculation procedure has been recently given for the binary Ti-Al system by the same authors in [11].

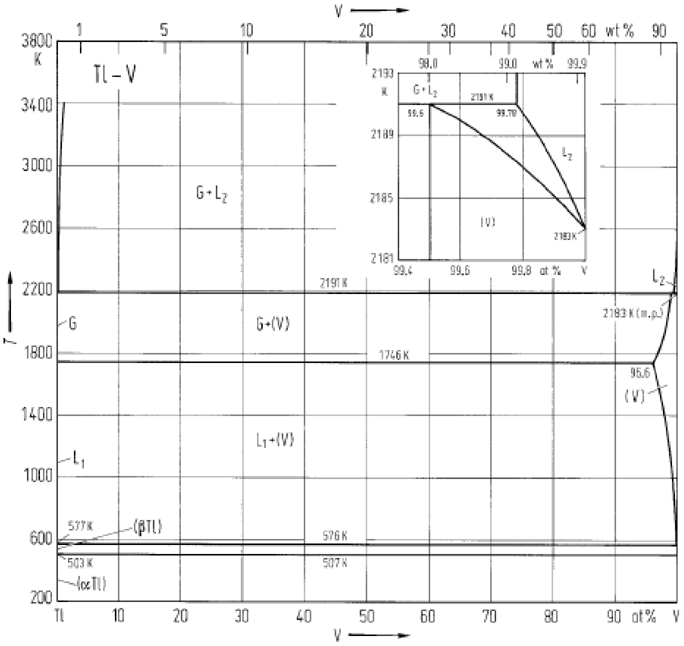

Fig.2. Phase diagram of Ti-V system

2. Results and Discussion

Thermodynamic analysis of binary Al-V and Ti-V systems was done using FactSage thermo-chemical software and databases at the temperatures of

2000K, 2073K, 2200K and 2273K.

The results obtained by calculation of thermodynamic quantities for the binary systems Al-V and Ti-V, including activities of both constitutive components, integral molar Gibbs energies of mixing and integral molar excess Gibbs energies at four investigated temperatures, are shown in Figs.3 and 4, and 5 and 6, respectively.

Strong negative deviation from Raoult law, indicating good mixing ability between constitutive components, is noticed for Al-V binary system. Temperature increase do not influence strongly to the change of activity values in the interval 2000-2273K. The values of integral molar Gibbs energies of mixing and integral molar excess Gibbs energies are both negative, but the minimum value for ΔG^M is far more negative about -21kJ/mol, while the minimum value for ΔG^{xs} is about -8kJ/mol. The change with temperature increase of these thermodynamic quantities is also slightly presented.

Considering the Ti-V binary system, the situation is different. Namely, noticeable positive deviation from Raoult law, indicating some demixing tendencies between constitutive components, is noticed. Temperature increase, in this case also, do not influence strongly to the change of activity values in the interval 2000-2273K. The values of integral molar Gibbs energies of mixing are negative, with minimum value of about -11kJ/mol and showing increase of negativity with the increase of temperature. On the other hand, integral molar excess Gibbs energies are positive, with the maximum value of about +2kJ/mol. There is a minimal change with temperature increase of this thermodynamic quantity, almost coinciding with the data at other temperatures.

Phase diagrams of the investigated binary Al-V and Ti-V systems, has also been investigated. The results obtained using FactSage, are shown in Fig. 7 and 8, respectively.

The phase diagram of binary Al-V system calculated using FactSage program is in accordance with literature data, presented in Fig.1, while there are some discrepancies in comparison of Ti-V calculated system and literature, given in Fig.2. Nevertheless, such results could be used in further investigations of mentioned binary systems based on vanadium and should be confirmed through some experimental work.

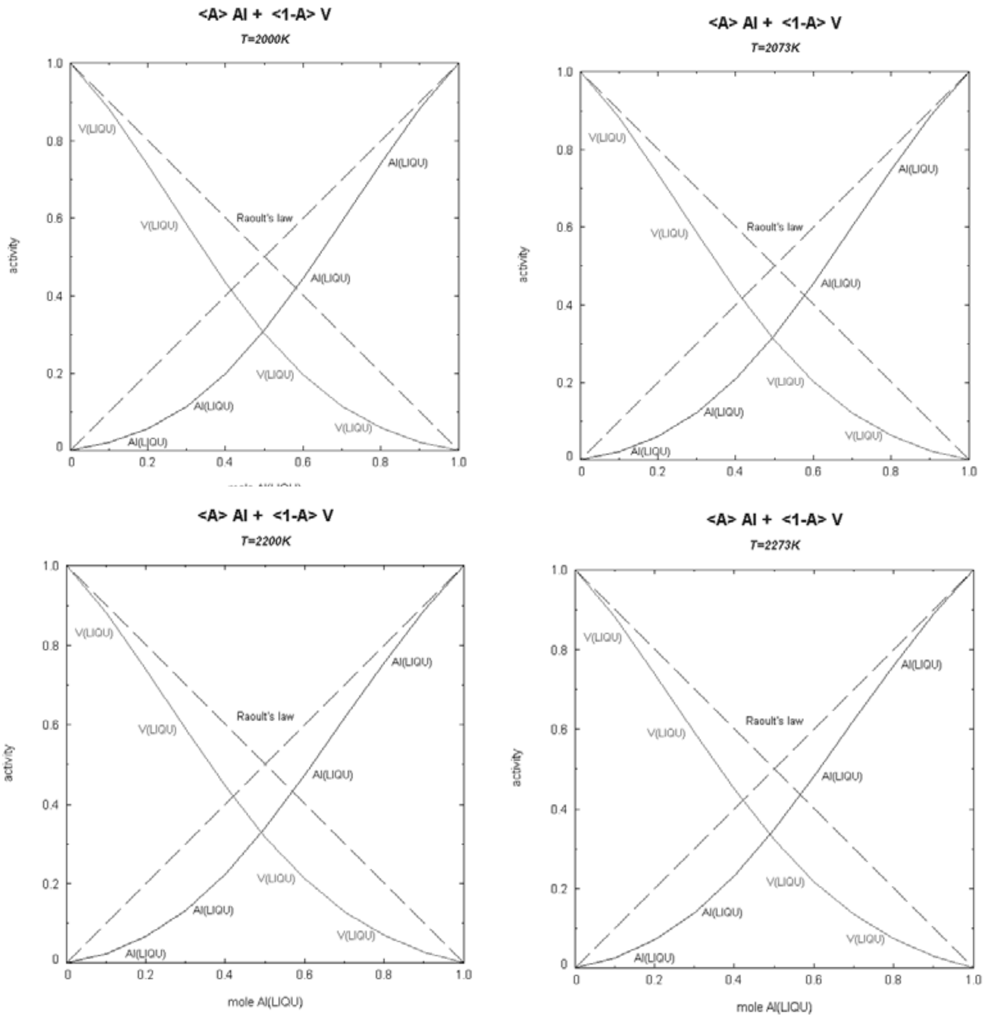

Fig.3. Activity of aluminum and vanadium in Al-V system at different temperatures

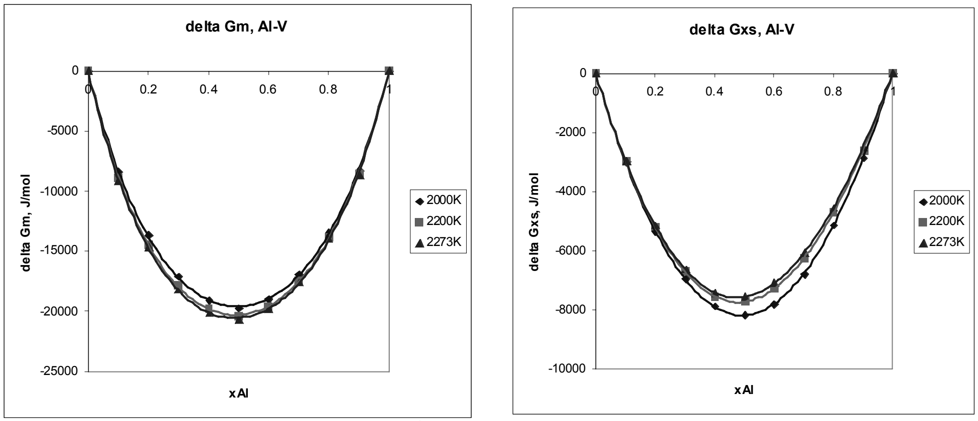

Fig.4. Integral Gibbs energy of mixing and integral excess Gibbs energy for Al-V binary system

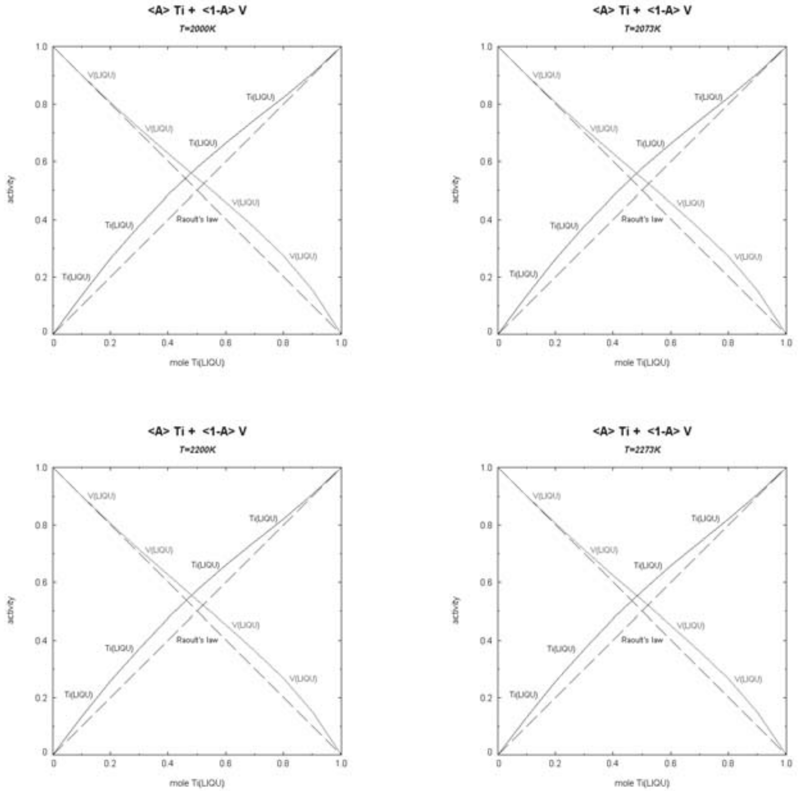

Fig.5. Activity of titanium and vanadium in Ti-V system at different temperatures

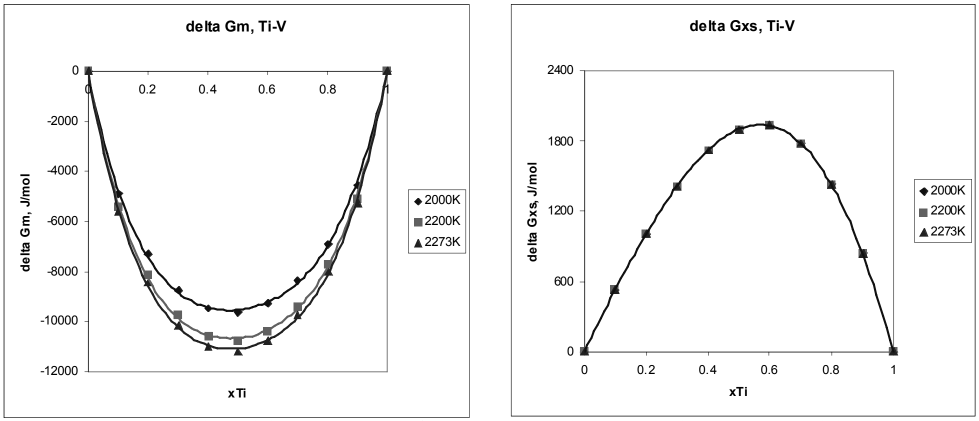

Fig.6. Integral Gibbs energy of mixing and integral excess Gibbs energy or Ti-V binary system

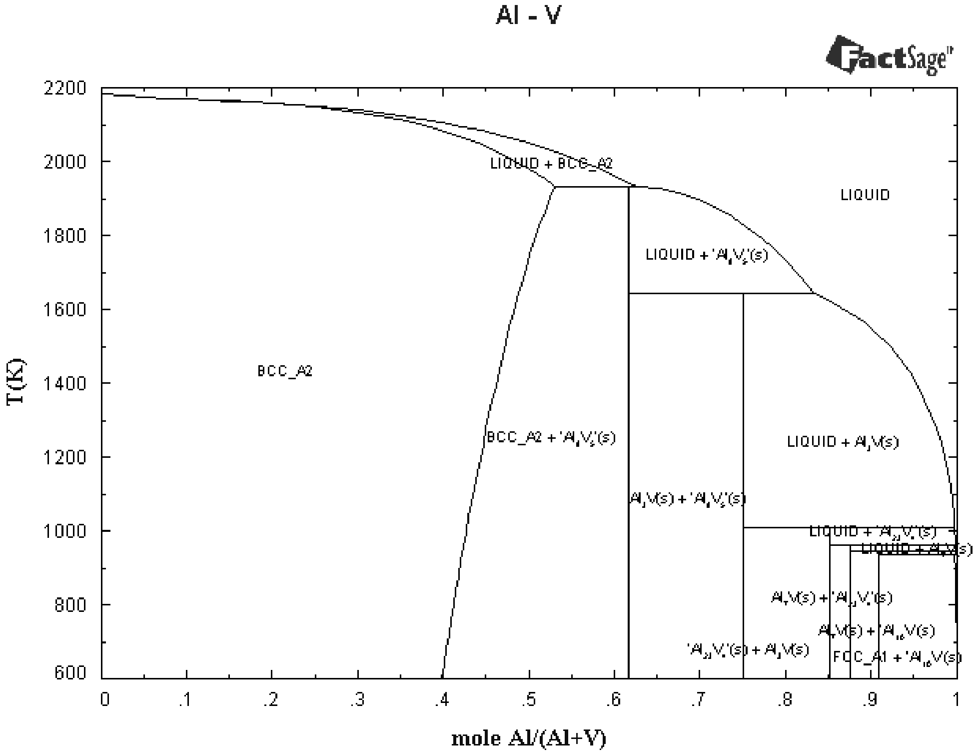

Fig.7. Phase diagram of Al-V system

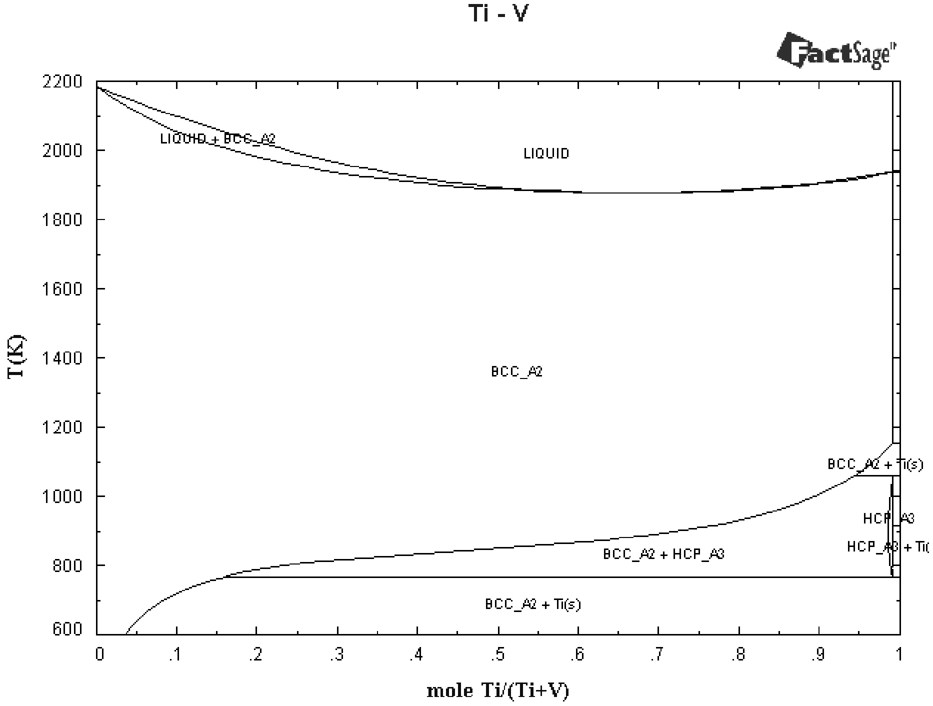

Fig.8. Phase diagram of Ti-V system

3. Conclusions

The thermodynamic properties of binary Ti-V and Al-V systems at the temperatures of 2000K, 2073K, 2200K and 2273K were calculated using the FactSage thermo-chemical software and databases. Having in mind that both systems have not been fully thermodynamically described, such obtained thermodynamic data may be useful for comparison with some future critical experimental results and for the further thermodynamic optimization of this system.

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