THERMODYNAMIC ANALYSIS OF Ti-Al, Ti-V, AND Al-V BINARY SYSTEMS

Ana Kostov[1], Dragana Živković[2], Bernd Friedrich[3]

[1] Copper Institute Bor, Serbia
[2] University of Belgrade, Technical Faculty Bor, Serbia
[3] RWTH University of Aachen, Institute for Process Metallurgy and Metal Recycling, Germany

ABSTRACT

Thermodynamic analysis of three binary Ti-based systems: Ti-Al, Ti-V, and Al-V 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 four different temperatures: 2000K, 2073K, 2200K and 2273K as well as calculated phase diagrams for the investigated binaries. The FactSage are used for all thermodynamic calculations.

Keywords: Binary systems Ti-Al, Ti-V, Al-V, thermodynamics, FactSage, phase diagrams

INTRODUCTION

The attractive mechanical properties, including the lightweight, strength to weight ratio, high ductility, and low thermal conductivity, result in more functional and comfortable use of titanium and titanium-based alloys. Titanium and its alloys have application in jet engines, airframes, industrial applications, space industry, power generation, chemical processing, petroleum, other industries, emerging applications, computer industry, automotive industry, geothermal power generation, and other various high temperature applications.

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. Unalloyed titanium shows low strength and poor wear resistance. Pure titanium undergoes a transition from a hexagonal close packed structure, α phase, to a body centered cubic structure, β phase. Alloying elements can be added to stabilize one or the other of these phases by either raising or lowering the transition temperatures. Elements such as Al, Ga, and Sn, with the interstitial elements C, O, and N stabilize α phase, resulting in alpha titanium alloy. On the other hand, elements such as V, Nb, Ta, and Mo, stabilize the β phase.

The Ti-based systems have long been a topic of interest because of the variability in the results reported by different researchers, especially for Ti-Al binary system. Ti-Al is one of the most investigated systems. This binary system is assessed by Murray [1] and by Kattner et al. [2] in the aim to obtain phase diagrams. These two diagrams exhibit several discrepancies not only in the equilibrium temperatures and the compositions but also in their phase relations. Particularly noticeable are the disagreement associated with the equilibria at high temperatures in Ti-Al aluminides, which are considered to arise mainly due to oxygen contamination. Kainuma et al. [3] have summarized such uncertainties and have carried out some investigations in the Ti-Al binary system. Because titanium aluminides are potencial candidates as high temperature light materials, a redetermination of the phase diagram in this region, using specimens with low levels of oxygen contamination, has become a priority. Kaufman and Nesor [4] reported their pioneering work on the calculation of the phase diagram in

the Ti-Al binary system, assuming all the intermetallic compounds to be of stoichiometric composition. Gros et al. [5] published a thermodynamic assessment of the phase equilibria between the liquid, β-Ti, α-Ti and α2-Ti3Al phases in the Ti-rich region of the diagram. The Gibbs energies of both the ordered α2-Ti3Al and disordered α-Ti phases were described by the unified two-sublattice model. Murray [6] also applied the same unified formalism to the Gibbs energy of the three ordered phases, while Ohnuma et al. [7] experimentally studied the phase equilibria between the Ti-rich solid phases, which were determined on specimens with carefully controlled low levels of oxygen contamination. At the end work of Tsakiropoulos and Shao [8] about phase transformations A2 into B2 and ω phase using microstructural data and nucleation theory coupled with phase equilibria calculations in Ti-Al-V system, as well as work of Quested and Dinsdale [9] about phase-diagram calculations by Calphad method and thermodynamic modeling software MTDATA for Al-rich alloys.

In the aim of contributing with some more data and approaches of thermodynamic description and determination of these systems, in this work the results of thermodynamic analysis in binaries Ti-Al, Ti-V, Al-V are done using FactSage thermo-chemical software and databases at 2000K, 2073K, 2200K and 2273K. Calculate of phase diagrams for the investigated system is done too.

RESULTS AND DISCUSSION

Results of thermodynamic analysis for the binary system Ti-Al are shown in figures 1 and 2, for the system Ti-V in figures 3 and 4, and for the system Al-V in figures 5 and 6. Phase diagrams of the investigated binary systems obtained by FactSage are shown in figures 7, 8 and 9, respectively.
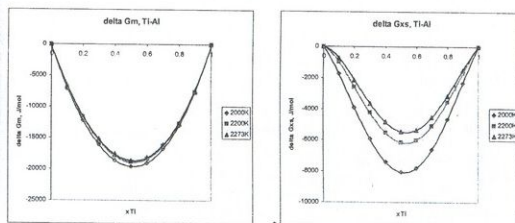

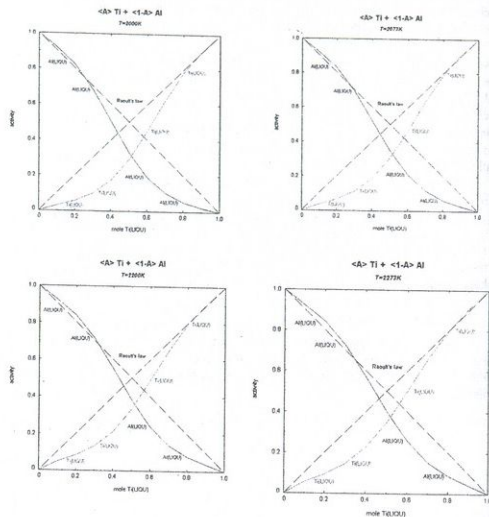Fig.1. Integral Gibbs energy of mixing and integral excess Gibbs energy for Ti-Al binary system

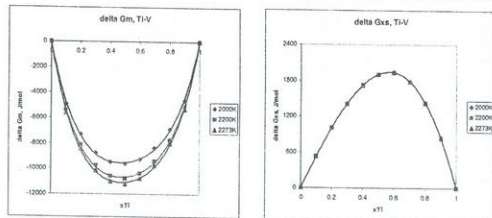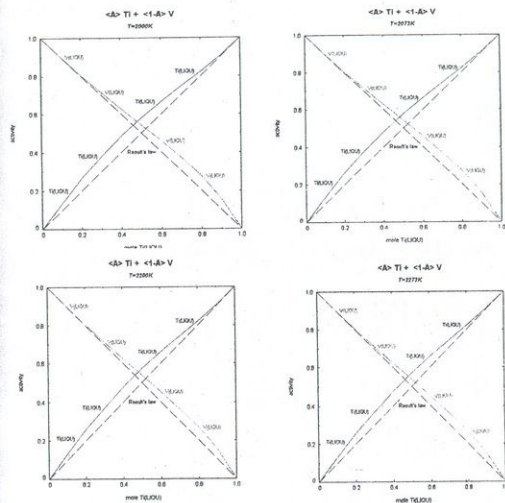Fig.2. Activity of titanium and aluminum in Ti-Al system at different temperatures

Fig.4. Activity of titanium and vanadium in Ti-V system at different temperatures

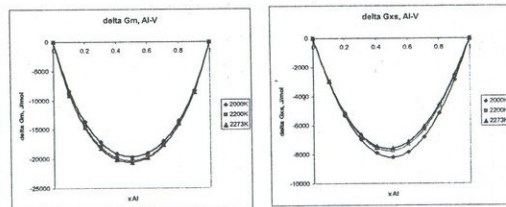Fig.3. Integral Gibbs energy of mixing and integral excess Gibbs energy for Ti-V binary system

Fig.5. Integral Gibbs energy of mixing and integral excess Gibbs energy for Al-V binary system
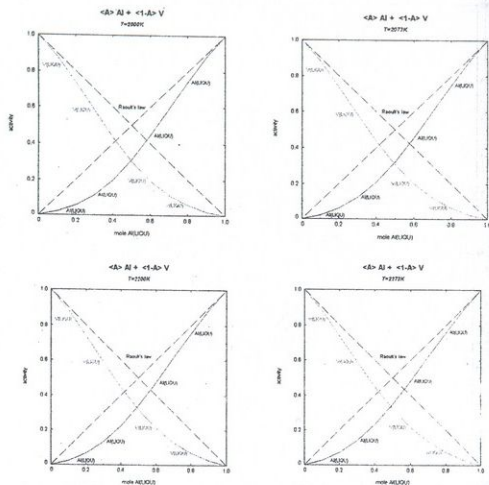
Fig.6. Activity of aluminum and vanadium in Al-V system at different temperatures
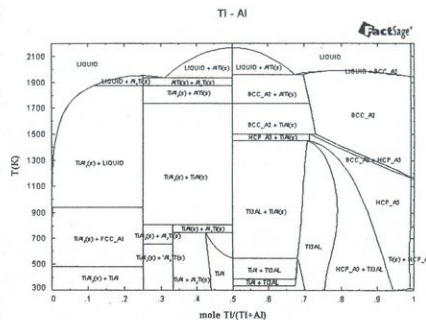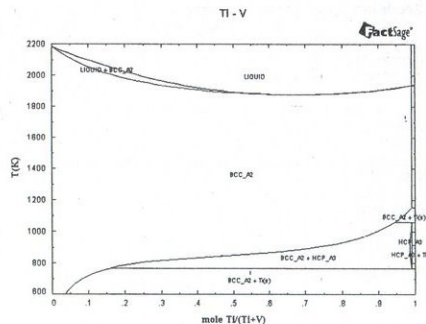

Fig.7. Phase diagrams of Ti-Al system

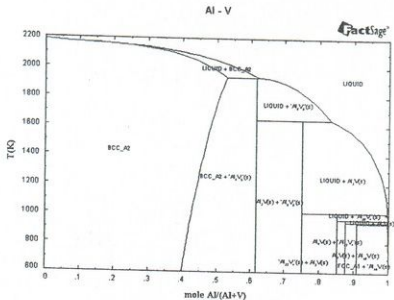

Fig.8. Phase diagram of Ti-V system

Fig.9. Phase diagram of Al-V system

CONCLUSIONS

The thermodynamic properties of binary systems: Ti-Al, Ti-V, Al-V at 2000K, 2073K, 2200K, and 2273K were calculated using the FactSage thermo-chemical software and databases.

Binaries Ti-Al and Al-V have negative values for integral excess Gibbs energy, while Ti-V system has positive values.

Enthalpies of mixing values indicate that strongest chemical interaction between the components exist between aluminum and vanadium and the weakest between titanium and vanadium.

According to obtained values for activities in Ti-Al and Al-V binaries, there is negative deviation of Raoult's law, while in Ti-V system is positive deviation of Raoult's law.

REFERENCES:

1. J.L.Murray (ed.), *Phase Diagrams of Binary titanium Alloys*, ASM International, Metal Park, OH, 1987, p.12.
2. U.R.Kattner, J.C.Lin and Y.A.Chang, *Metall. Trans. A*, 23 (1992) 2081.
3. R.Kainuma, M.Palm and G.Inden, *Intermetallics*, 2 (1994) 321.
4. L.Kayfman and H.Nesor, *Calphad*, 2 (1978) 325.
5. J.P.Gros, B.Sudman and I.Ansara, *Scripta Metall.*, 22 (1988) 1587.
6. J.L.Murray, *Metall. Trans. A*, 9 (1988) 243.
7. I.Ohnuma, Y.Fujita, H.Mitsui, K.Ishikawa, R.Kainuma and K.Ishida, *Acta Materialia*, 48 (2000) 3113.
8. P.Tsakiropoulos, G.Shao, *Materials Science and Engineering*, A375-377 (2004) 201.
9. T.E.Quested, A.T. Dinsdale, A.L.Greer, *Acta Materialia*, 53 (2005) 1323.