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Modeling Analyze from Titanium Alloy

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Abstract. Titanium and its alloys have been used a lot for its special and unique properties, and characteristics under different conditions [1]. When we want to use one of its alloys in aerospace industry, we have to assure that in these conditions the material will resist and keep its integrity [1,2]. We wanted to analyse a titanium based superalloy by modeling a routine and extracting information from it about the dependence between Gibbs free energy and the amount of weight from two components, titanium and aluminium, which is the second major element according to X-ray diffraction analysis. It was concluded that increasing Ti amount, or making the alloy richer on titanium, the system leads to a higher level of energy. The opposite behaviour happens with aluminium; increasing it, the energy of the system decreases which is great, once the equilibrium is obtained with lower levels of energy. Although the analysis had been done with a general database available in the software, it's possible to predict how the material will be influenced under several situations in a quick and reliable method.

Introduction

The increasing application of titanium alloys is due to their very good combination of mechanical properties and corrosion as well as erosion resistance. Its advantages include also low density, attractive strength-to-weight ratio and high-temperature capability [3]. Ti-based alloys were one of the first materials to which thermodynamics calculation were applied [4]. The first thermodynamic phase diagram calculated for Ti alloy was made in 1993 [5] and since then substantial advances have been done in terms of theoretical models definition, computer software and hardware, making possible higher evaluations of its alloys [4]. This visual representation of the state of a material as function of temperature, pressure and concentration of the components, turns to be a challenging task for system with more than three components, by the lack of sufficient experimental information. However, this graphical difficult is irrelevant for the calculation that can be customized by thermodynamics extrapolations and interaction functions using computational interaction [5].

The computer modeling and simulation is attractive and highly desirable because it's a way to reduce costs and time consuming, variables inherent for empirical studies [3].

The compounds existed for Ti-alloys, like α_2-Ti_3Al or γ-TiAl, have considerable interest, especially because of its influence towards applicability at higher temperatures regimes, and oxidation as well burn resistance are desirable [4]. Saunders and Chandrasekaran published a study about the importance of light elements (O, C, N) as well those with low amount in the alloy description to accurate the representation of the phase equilibria as well as provide information about the forms when considering mechanical properties [7]. There are strongly dependence between the microstructure and mechanical properties with the alloy's chemistry, requiring this way a multicomponent phase equilibrium information [8].

Thermodynamic models of alloy system are needed for interpreting and predicting the behavior of the phase formation by novel processing techniques. Rare thermodynamic data exists to fully formulate these models.

The roots of CALPHAD (Computer Calculation of Phase Diagrams) approach lies in the mathematical description of thermodynamic properties of the phases, this method is part of software packages such as *Thermo-Calc* [3]. With the development of thermodynamic modeling approach, only a few experiments are required to describe the system and its properties [5]. The theoretical basis of thermodynamics calculations rest on the fact that the phase boundary is a result of stability competition between the phases, described by Gibbs energy. The software's used works towards minimizing this energy and find the equilibrium state for the system [8]. For a binary metallic phase, the free energy is described by the equation

$$G^i = G^i_1 x_1 + G^i_2 x_2 + RT\,(x_1 \ln x_1 + x_2 \ln x_2) + G^i_{ex} \quad (1)$$

where G^i_1 and G^i_2 are the lattice stabilities (i.e., reference to chemical potentials) of pure elements; x_1 (=1 – x_2) is the molar fraction for component 1; G^i_{ex} is the excess free energy of mixing of phase *i* [9]. This formula can be extended to a multicomponents analysis.

The aim of this work is to model correlations and phenomena of processing-microstructure-property for titanium alloy, and compare those results with experimental ones validating the analysis done computationally.

Experimental Procedure

There are different equilibrium amounts of α (hcp) and β (bcc) phases as well as equilibrium compositions of both phases depending on the conditions input to the system. Phase equilibria was calculated for the Ti-alloy, which composition is presented on Table 1, with *Thermo-Calc* software.

Table 1 – Composition of the Ti-alloy studied.

Element	O	Al	V	Cr	Co	Ni	Y	Zr	Ti
%wt	2,08	5,04	4,74	0,49	1,08	0,91	0,06	1,94	balance

This alloy was chosen because it was widely studied and evaluated for creep applications, showing great responses compared to conventional ones [10]. Thermodynamic calculations were performed to calculate the phase equilibria using SSOL4 (solid solution version 4) database.

SEM analysis was done following the metallographic standard procedure with a surface polishing with Kroll solution to reveal the microstructure and using backscattered electron mode.

Results

A first calculation was done in order to determine the temperature of β-transus resulting as 1021 K (748°C); it's lower than pure Ti (1156 K or 883°C) because of the high amount level of β-stabilizers presented in this alloy. Except for oxygen and aluminum, the other metals provide a reduction on temperature transition, mainly V that can reduce until room temperature if added in sufficient concentration. A comparison was made by calculus from Yoltan's formula, equation (2):

$$\beta_T = 882 + \Sigma b_j X_j \quad (2)$$

where b_j is a constant for a particular element and X_j is the weight percent of the element present in the alloy.

The formula resulted in 790°C for β_T, showing a slightly difference between the methods. It's possible that this almost 42° difference comes because of the value of the constants b_j adopted for the elements, which can vary from publishers. In Fig. 1 it's shown the influence of bcc phase fraction according to temperature generated from *Thermo-Calc* calculation. At around 620°C there are equivalent amount between bcc and hcp phases.

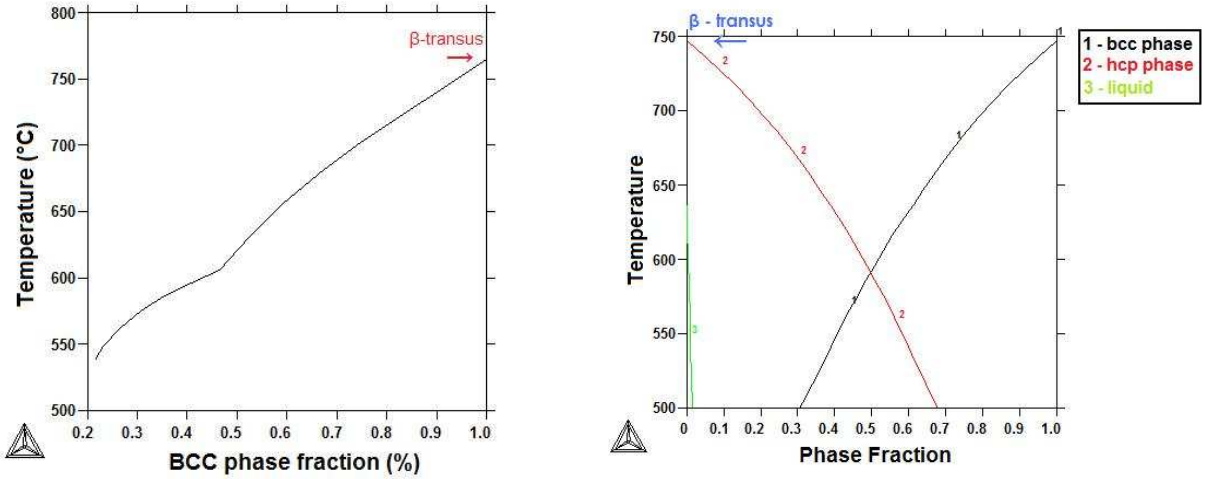

Figure 1 – Influence of the temperature on the amount of (a) exclusive bcc phase fraction, and (b) bcc, hcp and liquid phases.

It was possible to determine the isothermal section for 500°, 600° and 700°C for the alloy (Fig. 2), and study the evaluation towards temperature of the bcc, hcp and liquid phases.

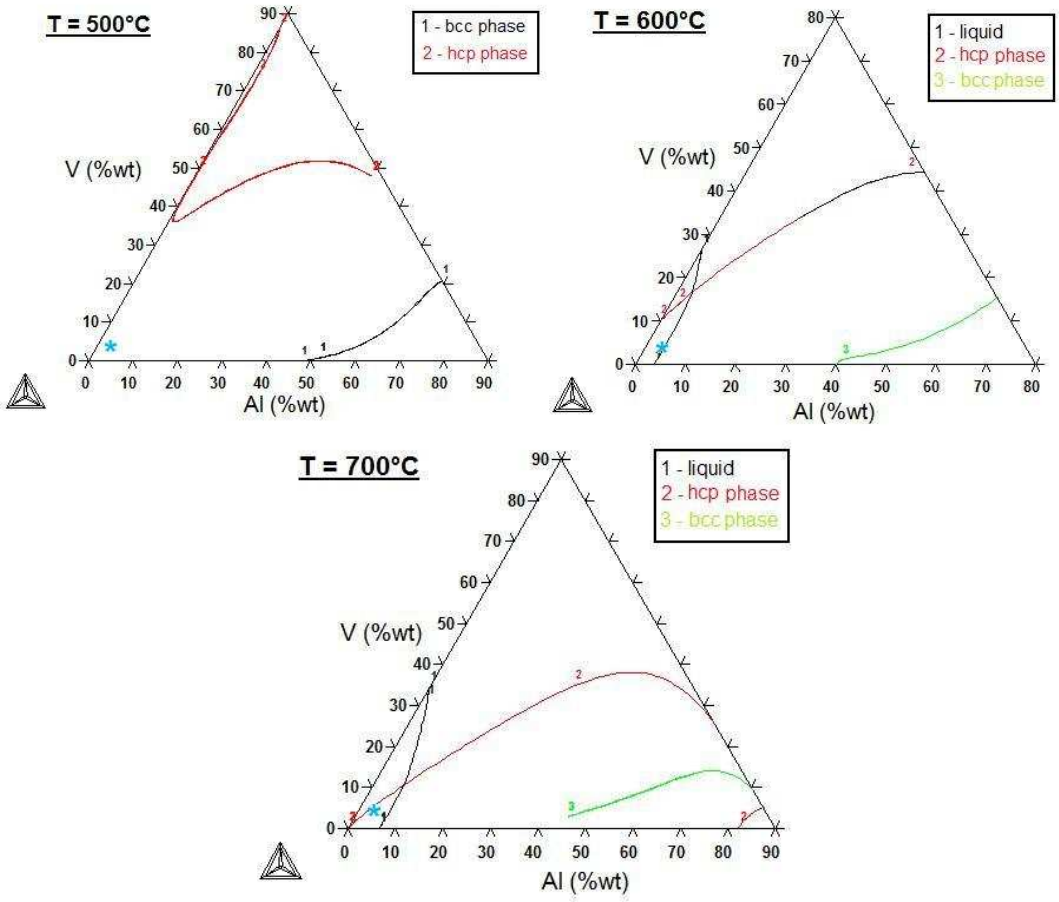

Figure 2 – Isothermal sections for the alloy at 500°, 600° and 700°C. The asterisk represents the position of the alloy studied.

From Fig. 2 it is possible to see that liquid phase appears before 600°C at the Ti rich side. At higher temperatures, the liquid phase increases its field and there are some changes on the curvature of bcc and hcp phases, because of the stability of them.

A SEM analysis was done for the alloy that was submitted under creep tests. The microanalysis can be shown on Fig. 3.

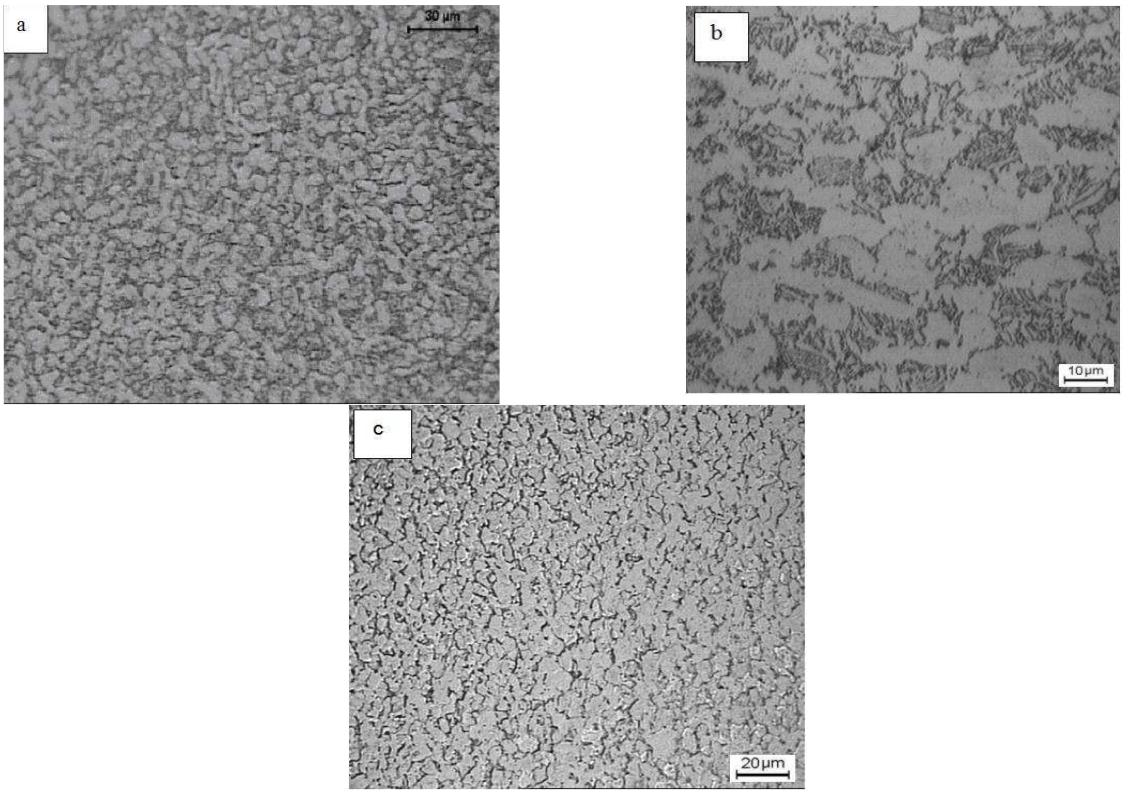

Figure 3 – Micrographs from SEM for the conditions (a) as provided, and after creep test under (b) 600° and (c) 700°C.

From Fig. 3 (a), grains of α-phase (hcp) can be seen and dark regions indicates the presence of β-phase (bcc) around the grain boundary, in concordance to Fig. 2, it's a two phase region. At (b) and (c), there are growing of α-phase and dissolution of β, which was continuous at (a); this effect was also predicted from computational results, Fig. 2, at these temperature there are presence of liquid with α-phase, the cooling provides the transformation of liquids into α and β-phases in the α-matrix.

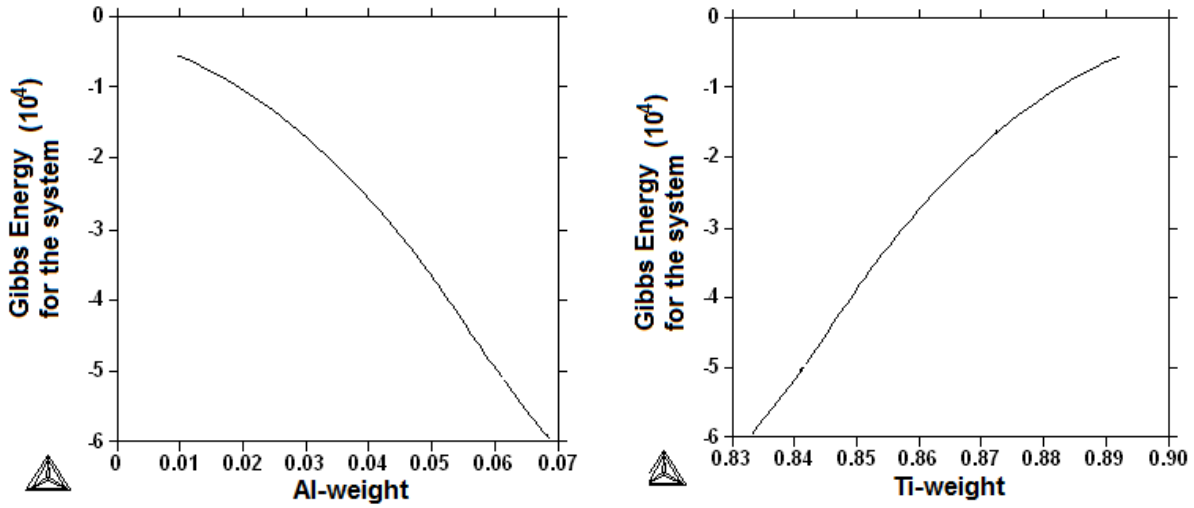

Figure 4 – Influence of the element on stability of the alloy at high temperatures (a) Al, and (b) Ti

An analysis of the Gibbs-free energy can be done and its dependence on the element weight amount. On Fig. 4 is possible to compare these results considering titanium and aluminum influence.

The increase of Al promotes a diminishing on Gibbs energy, which provides a higher stability of the high temperature phases, the opposite behavior happens when considering Ti. If the purity of the alloy increases, there are less chance to promote a stability at room temperature of the phases, there would be none metastable phases or unexpected ones.

The effect of Al content in the alloy can be also predicted using *Thermo-Calc*, this metal is responsible itself to increase the temperature that the alloy can be used. Although this element limits to around 10%wt quantity, higher values can't be performed in the alloy.

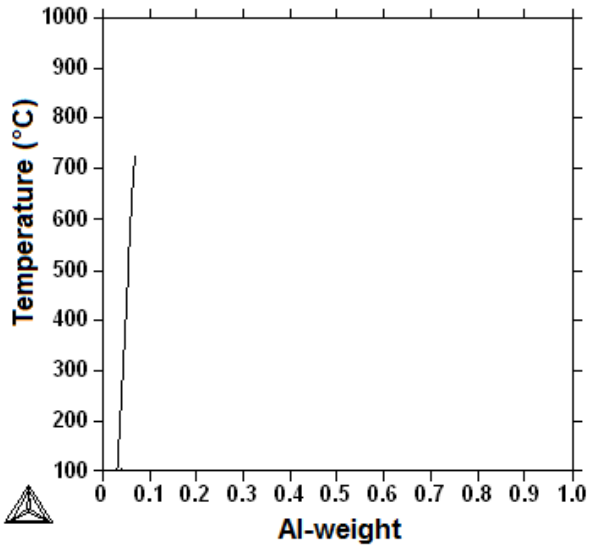

Figure 5 - Effect of the aluminum content over the temperature of the alloy.

Conclusion

It clear that the use of CALPHAD method is a powerful tool in the prediction and understanding of fundamental features of conventional Ti-alloys, and it can also be extended to correlated areas of study. The success of any thermodynamic calculation depends on the availability of reliable thermodynamic database. Much progress has been made in the description of model descriptions and further advances seem to come up according to the advances on studies and scientific investigation of the system. The *Thermo-Calc* is a powerful tool to describe well the properties of Ti-alloys, such as β-transus, phase diagram description and stability.

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