Computational Materials Science 111 (2016) 41–46

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Analysis of the effect of alloy elements on allotropic transformation in titanium alloys with the use of cohesive energy

Cheng Lin [a,*], Guili Yin [a], Yongqing Zhao [b], Jianzhong Wang [a]

[a] College of Materials Science and Engineering, Liaoning University of Technology, Jinzhou, Liaoning 121001, China
[b] Northwest Institute for Nonferrous Metal Research, Xi'an, Shanxi 710016, China

ARTICLE INFO

Article history:
Received 19 June 2015
Accepted 31 August 2015
Available online 19 September 2015

Keywords:
Titanium alloys
Phase transformations
Modeling
Thermodynamics
Electronic band structure

ABSTRACT

A simple model to account for the effect of alloy elements on allotropic transformation in titanium alloys is described using the cohesive energies calculated with the self-consistent bond length difference (SCBLD) method in the empirical electron theory (EET) of solids and molecules. The results indicate the total cohesive energy ($S\bar{E}_c$) as well as cohesive energy difference ($\Delta\bar{E}_c$) for α and β phases can be used to investigate the influence of alloying elements on the allotropic transformation of β to α. Moreover, the deterministic model agrees well with the experimental results.

1. Introduction

Allotropic transformation in titanium alloys is a fundamental to investigate microstructure and property of alloys [1]. Moreover, allotropic transformation is significantly depended on the alloying elements added into pure titanium [2]. Prior researches [3–6] have shown that some of the elements present in titanium alloys are α-stabilizers (e.g., Al); some are neutral elements (e.g., Zr, Hf and Sn) which only have a minor influence on the β-transus temperature; and some are β-stabilizers. Among β-stabilizers, there are two types of equilibrium phase diagrams [6], i.e., the isomorphous and eutectoid decompositions of β phase. The former includes Mo, V, Ta, and Nb, and the latter includes Cr, Mn, Fe, Co, Ni and Cu. Although the fundamental researches related to the allotropic transformation in titanium alloys, such as the orientation relationship (OR) [7] and the crystallography associated with OR [8], have been investigated in depth, little attention has been paid on the detail mechanism which accounts for the effect of alloying elements on allotropic transformation at the level of electron structure because the advanced electron structure calculation methods such as density functional theory (DFT) still have a difficulty to deal with the electron structure and properties of the actual solid solutions alloyed with different elements [9–12]. Nevertheless, the empirical electron theory (EET) of solids and molecules [13,14], which is not needed to explore approximate solutions to the Schrödinger equations of the system as well as not needed to construct advanced electron density functionals, has special superiority in the investigation of complicated alloy systems in spite of some disadvantages [15,16]. In EET, the atom state, electron structure, and systematic energy can be exhibited in real space rather than reciprocal space through implementing the bond length difference (BLD) method on the base of four basic assumptions. Nowadays, EET has been widely applied to study many properties of solids and molecules [17–25].

In this present paper, we systematically investigated the influence mechanism of alloying elements on allotropic transformation in titanium alloys at the electron structure level with the use of the cohesive energies calculated with the self-consistent bond length difference (SCBLD) method [15,16] based on EET. The previous results [24,25] based on the BLD method have shown that the stability of the β phase, the separation of β phase, and the eutectoid reaction of the β-phase enrichment in β-stabilizing elements can be associated with the valence electron structure parameters of β phase. However, many phenomena (e.g., the distinction between neutral and isomorphous elements) are not disclosed clearly only by considering the single β phase because the allotropic transformation of β to α simultaneously deals with the decomposition of β phase, the construction of α phase and the diffusive motion of atoms between α and β phases. Therefore, it is necessary to comprehensively and deeply understand the influence mechanism of alloying elements on the allotropic transformation of β to α at the atom or electron structure levels.

* Corresponding author.
E-mail address: Cheng_lin1979@163.com (C. Lin).

http://dx.doi.org/10.1016/j.commatsci.2015.08.060
0927-0256/

2. Calculation method

2.1. Calculation models of EET

In binary α (or β) solid solution of Ti alloy, the hcp-structured α phase (or bcc-structured β phase) is considered to be composed of pure α-Ti (or β-Ti) structure unit (cell) and the α-Ti–M (or β-Ti–M) structure unit (alloy M into pure Ti cell). In view of the randomness and indeterminacy in the position and amount of the alloying atoms dissolved in α or β phases, the calculation models supposed in our previous investigations [17,18] were adopted in the present work. Fig. 1 shows the atom arrangement and bond distribution for α and β phases with and without alloying atom M. When the alloy atom M dissolves into α or β phases, it is supposed that a kind of mixing atom that is composed of $(1-x)$Ti and xM atoms (x, at.%) occupies the lattice points in a cell; here, x equals to 1/6 and 1/4 for α-Ti–M and β-Ti–M structure units, respectively. Thereby, the SCBLD analysis and the calculation of cohesive energy are needed to carry out for α-Ti, α-Ti–M, β-Ti and β-Ti–M structure units, respectively.

2.2. SCBLD analysis

The main equations for the SCBLD method in EET are given in Ref. [15]. Moreover, the SCBLD analysis for the pure α-Ti and β-Ti structure units can be proceeded as the solving process (Fig. 2) in Ref. [15]. Although the SCBLD analysis procedures for the α-Ti–M and β-Ti–M structure units are the same as the ones of α-Ti and β-Ti structure units, the character parameters of mixed atoms are different from the ones of pure Ti atom in α-Ti or β-Ti structure units. The character parameters of mixed atoms in the α-Ti–M and β-Ti–M structure units, such as the single-bond radius $R(1)$, covalent electron number n_C, lattice electron number n_l, magnetic electron number n_m, dumb pair electron number n_d, bond-forming ability f, and shielding factor b, are the weighted average of the component elements in the solid solution.

For α-Ti–M structure unit, there are

$$\left.\begin{array}{l} R_X(1)=\frac{5}{6}R_{Ti}(1)+\frac{1}{6}R_M(1),\ n_C^X=\frac{5}{6}n_C^{Ti}+\frac{1}{6}n_C^M,\ n_l^X=\frac{5}{6}n_l^{Ti}+\frac{1}{6}n_l^M \\ n_m^X=\frac{5}{6}n_m^{Ti}+\frac{1}{6}n_m^M,\ n_d^X=\frac{5}{6}n_d^{Ti}+\frac{1}{6}n_d^M,\ f_X=\frac{5}{6}f_{Ti}+\frac{1}{6}f_M \\ b_X=\frac{5}{6}b_{Ti}+\frac{1}{6}b_M \end{array}\right\} \quad (1)$$

For β-Ti–M structure unit, there are

$$\left.\begin{array}{l} R_X(1)=\frac{3}{4}R_{Ti}(1)+\frac{1}{4}R_M(1),\ n_C^X=\frac{3}{4}n_C^{Ti}+\frac{1}{4}n_C^M,\ n_l^X=\frac{3}{4}n_l^{Ti}+\frac{1}{4}n_l^M \\ n_m^X=\frac{3}{4}n_m^{Ti}+\frac{1}{4}n_m^M,\ n_d^X=\frac{3}{4}n_d^{Ti}+\frac{1}{4}n_d^M,\ f_X=\frac{3}{4}f_{Ti}+\frac{1}{4}f_M \\ b_X=\frac{3}{4}b_{Ti}+\frac{1}{4}b_M \end{array}\right\} \quad (2)$$

Table 1 shows the covalent bond name (CBN), the experimental bond length (EBL), the equivalent bond number (EBN), and the electron conservation equation (ECE) for the above crystal structures, respectively. These calculated parameters and the measured lattice constants are inputted into the calculation software of SCBLD method, the calculated lattice constants can be obtained, as shown in Tables 2 and 3.

2.3. Calculation of cohesive energy

The calculation formulas of cohesive energy $\overline{E}_C$ [16] in EET can be expressed as

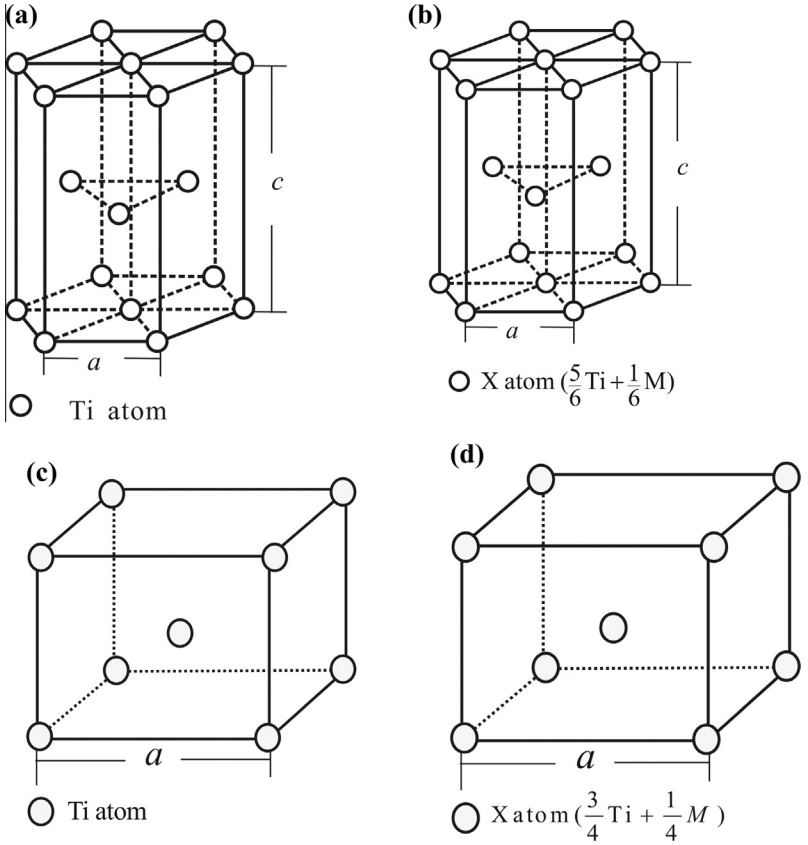

Fig. 1. The atom arrangement and bond distribution for α and β phases [17,18]. (a) α-Ti structure unit; (b) α-Ti–M structure unit; (c) β-Ti structure unit; (d) β-Ti–M structure unit.