

A simple model to ascertain the initial formation concentration of athermal ω phase in titanium alloys



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ABSTRACT

This article describes a simple model to ascertain the initial formation concentration of athermal ω phase in titanium alloys through the self-consistent bond length difference (SCBLD) method in the empirical electron theory (EET) of solids and molecules. The results indicate that the calculated cohesive energies can be used to determinate the initial formation concentration of athermal ω phase in titanium alloys in combination with the critical concentration C_k . Moreover, the deterministic model accords well with the experimental results, with the average value of absolute relative errors of 4.90%.

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1. Introduction

Titanium and its alloys are important structural materials and have been used widely in lighter aircrafts due to their high specific strength and acceptable ductility and toughness [1,2]. Moreover, their phase transformations have attracted considerable interest in the recent past [3–5]. The phase transformations in titanium alloys can be classified into two kinds in the light of atom motion patterns. One kind is dominated by diffusion, such as allotropic transformation [6], eutectoid reaction [7], β separation [8]; the other kind is dominated by displacive movement, such as martensitic transformation [9] and athermal ω transformation [10]. However, athermal ω transformation is different from the martensitic transformation in terms of transformation mechanism and microstructure morphology [11–13]. Its transformation mechanism is not the cooperative atom motion within the (1 1 0) plane of β phase but the result of the atom collapse of (1 1 1) plane [14–16]. Additionally, the morphology of athermal ω phase has a separation between particles [11], which is different from the character of martensitic morphology (plate-like).

This metastable ω can be formed in titanium alloys in which the concentration of β -stabilizing elements is close to the critical concentration (C_k) during quenching from the high-temperature single β (bcc) phase field [6]. Nevertheless, the initial formation concen-

tration of athermal ω is still not obtained in theory. Moreover, the effect of alloy elements on athermal ω has also not been investigated clearly at electron structure level. Thereby, the empirical electron theory (EET) of solids and molecules [17,18], established in 1978 by Yu on the base of Pauling's valence bond theory and Hume-Rothery's electron concentration theory, is used to investigate the initial formation concentration of athermal ω . In this theory, we can present the electron structure, atom state, and systematic energy for the considered systems by conducting the self-consistent bond length difference (SCBLD) method [19]. At present, although EET is not the mainstream of electron structure simulation, this theory has been widely used to investigate solid solution, compound, electrical conductivity, magnetic property, mechanical property, strengthening mechanism and phase transformation, surface energy of elements, texture formation mechanism, etc. [19–40]. In our opinion, the EET concept will be broadly adopted on an international scale with the increase in the outstanding results based on EET.

The novel features of this study are as follows. The studied results exhibit the necessity of alloying treatment to the formation of athermal ω ; the complex influences of alloying elements on athermal ω are disclosed at the electron structure level; the initial formation concentration of athermal ω in titanium alloys is determined in the combination with C_k .

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2. Calculation method

2.1. SCBLD analysis of EET

The athermal ω phase in titanium alloys has the non-close-packed hexagonal lattice (Fig. 1(a)), its lattice constants are $a = b = 0.4607$ nm, $c = 0.2821$ nm. When the alloy atom M dissolves into ω -Ti cell, the amount and position of alloy atom M is random and indeterminate. Therefore, in the light of the calculation models supposed in our previous investigations [28,29,31], we suppose that only Ti2 atoms can be replaced in ω -Ti cell as well as consider that a kind of mixing atom that is composed of $\frac{(6-x)}{6}$ Ti2 and $\frac{x}{6}$ M atoms ($0 < x \leq 6$) occupies the lattice points of Ti2 atoms, as shown in Fig. 1(b).

The main equations for the SCBLD method in EET are given in Ref. [19], and its solving process can be seen in Fig. 2. The SCBLD analysis for the ω -Ti structure unit was conducted in Ref. [32]. Although the SCBLD analysis procedures are the same for the ω -Ti and ω -Ti-M structure units, they have distinct atom character parameters. In ω -Ti-M structure unit, the characteristic parameters for the mixed atoms consisting of Ti2 and M, 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 Ti2 and M atoms, i.e.,

$$\left. \begin{aligned} R_x(1) &= \frac{(6-x)}{6} R_{\text{Ti2}}(1) + \frac{x}{6} R_M(1) \\ n_c^x &= \frac{(6-x)}{6} n_c^{\text{Ti2}} + \frac{x}{6} n_c^M \\ n_m^x &= \frac{(6-x)}{6} n_m^{\text{Ti2}} + \frac{x}{6} n_m^M \\ n_d^x &= \frac{(6-x)}{6} n_d^{\text{Ti2}} + \frac{x}{6} n_d^M \\ f_x &= \frac{(6-x)}{6} f_{\text{Ti2}} + \frac{x}{6} f_M \\ b_x &= \frac{(6-x)}{6} b_{\text{Ti2}} + \frac{x}{6} b_M \end{aligned} \right\} \quad (1)$$

The necessary calculation parameters for ω -Ti and ω -Ti-M structure units, such as the covalent bond name (B_x), the experimental bond length (D_{nz}^{u-v}), the equivalent bond number (I_x), and the electron conservation equation, are given in Table 1, respectively. Inputting these calculated parameters and the measured

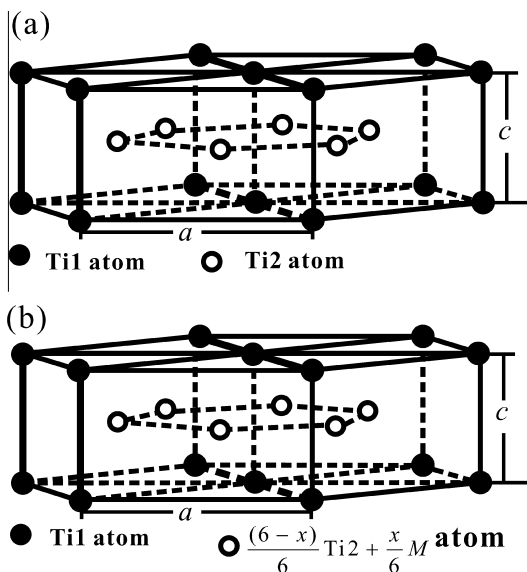


Fig. 1. Atom arrangement for ω phase. (a) ω -Ti structure unit; (b) ω -Ti-M structure unit.

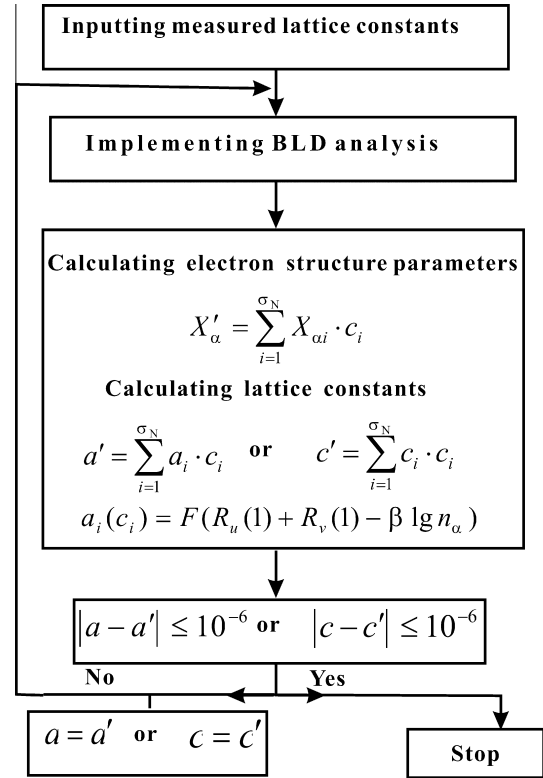


Fig. 2. Solving process of the SCBLD method [19].

lattice constants into the calculation software of SCBLD method, we can obtain the valence electron structure parameters and the calculated lattice constants for ω -Ti and ω -Ti-M structure units.

2.2. Calculation of cohesive energy

In terms of the calculation formulas in Ref. [20], the cohesive energy \bar{E}_c of ω -Ti and ω -Ti-M structure units can be calculated, i.e.,

$$\left. \begin{aligned} \bar{E}_c &= b \left\{ \sum_{\alpha} \frac{I_{\alpha} n_{\alpha}}{D_{n\alpha}} f + \frac{n_l}{D} f' + km^{3d} - CW \right\} \\ \bar{E}_c &= \sum_{i=1}^{\sigma_N} \bar{E}_{Ci} \cdot C_i \end{aligned} \right\} \quad (2)$$

where the meaning of above calculation parameters has been given in Refs. [19,20]. According to the solving process given in Fig. 3, we can obtain cohesive energies and their statistical value \bar{E}_c for ω -Ti and ω -Ti-M structure units.

3. Results and discussion

Referring to the definition of cohesive energy given in Ref. [31] that the cohesive energy equals to the released energy to form solids from free atoms or equals to the absorbed energy to form free atoms from solids, we can conclude that both the large and small cohesive energies are not in favor of the formation of athermal ω . Although the large cohesive energy can enhance the stability of athermal ω , the formation of athermal ω is quite difficult. On the contrary, the structure unit with small cohesive energy is easy to form, but this structure unit is also destroyed easily. Therefore, the appropriate cohesive energy is an important factor for the occurrence of athermal ω in titanium alloys. However, it is still difficult to verify the cohesive energies of solid solutions in both experiment and theory. Thereby, the cohesive energies, associated with C_k , can be selected as a vital criterion to investigate the formation of athermal ω because the athermal ω precipitates can be

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