A Cluster-Formula Composition Design Approach in β-Ti Alloys

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Abstract: Cluster-plus-glue-atom model was proposed to deal with short-range-order structures in quasicrystals, metallic glasses, and solid solution alloys. In this model, the characteristic short-range-order structure is simplified into a local structural unit, where the atomic interactions are best satisfied locally, covering only the nearest neighbors (or cluster for short) and a few outer-shell atoms (called glue atoms). The unit is then formulated as [cluster](glue atoms), indicating that one cluster is matched with a few glue atoms. In this paper, a novel Ti-4.13Al-9.36V (wt. %) alloy with cluster-formula of 4[Al-Ti_{12}](AlTi_2)+12[Al-Ti_{14}](V_2Ti) was designed based on the cluster-formula of Ti-6Al-4V. Compared to Ti-6Al-4V, the tensile strength of Ti-4.13Al-9.36V alloy increased to 1045MPa, by 13%, and the ductility increased to 13.2%, by 164%.

Keywords: Cluster-plus-glue-atom model, β-Ti alloys, composition design

1 Introduction

Titanium alloys are widely used due to their good properties in strength, toughness, formability, weld-ability, corrosion resistance and biocompatibility [1]. However, limited by the missing model for chemical short-range-ordering, their composition rule is unresolved for long which has hindered the development of high-performance Titanium alloys. Cluster-plus-glue-atom model is an effective method to describe chemical short-range-ordering [2]. In this model, the chemical short-range-ordering is simplified into a local structural unit, where the atomic interactions are the best satisfied locally, covering only the nearest neighbors (or cluster for short) and a few outer-shell atoms (called glue atoms). The unit is formulated as [cluster](glue atoms)x, indicating that one cluster is matched with a few glue atoms. The model has been successfully used as an effective alloy composition design method in Titanium alloys [3, 4]. In this paper, according to the cluster formula of Ti-6Al-4V alloy, the β-Ti alloys have been designed.

2 Composition design

In our previous work, the chemical units of α and β phases in Ti-6Al-4V were revealed which are [Al-Ti_{12}](AlTi_2) and [Al-Ti_{14}](V_2Ti), respectively. Being analogous to the atomic resonance theory, the stacking unit of Ti-6Al-4V alloy can be calculated to contain 17 hard spheres, and the ratio of the α phase and β phase structural units only meets 12: 5. Therefore, the cluster-plus-glue-atom model of Ti-6Al-4V is 12[Al-Ti_{12}](AlTi_2)+5[Al-Ti_{14}](V_2Ti) [5].

Considered the β cluster formula of Ti-6Al-4V is taken as solvent, and α cluster formula is taken as solute, the cluster formula of novel alloy can be expressed as [{β}-{α}$_{12}$]{α}$_x${β}$_y$. x and y are the number of glue clusters of {α} and {β}, respectively. The value of x and y can be calculated by the following equation:

$$x \cdot R_{\alpha/\beta}^3 + y = 2.03 \cdot (R_{\alpha/\beta} + 1)^3 - R\alpha/\beta^3 - 12 \quad (1)$$

where, $R_{\alpha/\beta}$ is the radius ratio of the hard sphere of α and β phases cluster formula. Using the hard sphere radius of α and β phases of 0.367 nm and 0.379 nm, respectively, the above equation goes to:

$$1.154x + y \approx 4.309 \quad (2)$$

The solutions of Eq. (2), the closest to integers, are x=3 and y=0, meaning that the novel alloy cluster formula is 4[Al-Ti_{12}](AlTi_2)+12[Al-Ti_{14}](V_2Ti), and the composition is Ti-4.13Al-9.36V (wt.%).

3 Mechanical properties of designed Titanium alloys

Figure1 displays the microstructure of both alloys contained prior-β equiaxial grains. The width of the prior-β equiaxial grains decreases as the cluster ratio changes from 12:5 to 4:12. The microstructure within the prior-β equiaxial grains consists of Widmanstätten acicular α phase in both alloys, but as the cluster ratio changes from 12:5 to 4:12, α phase content decrease.

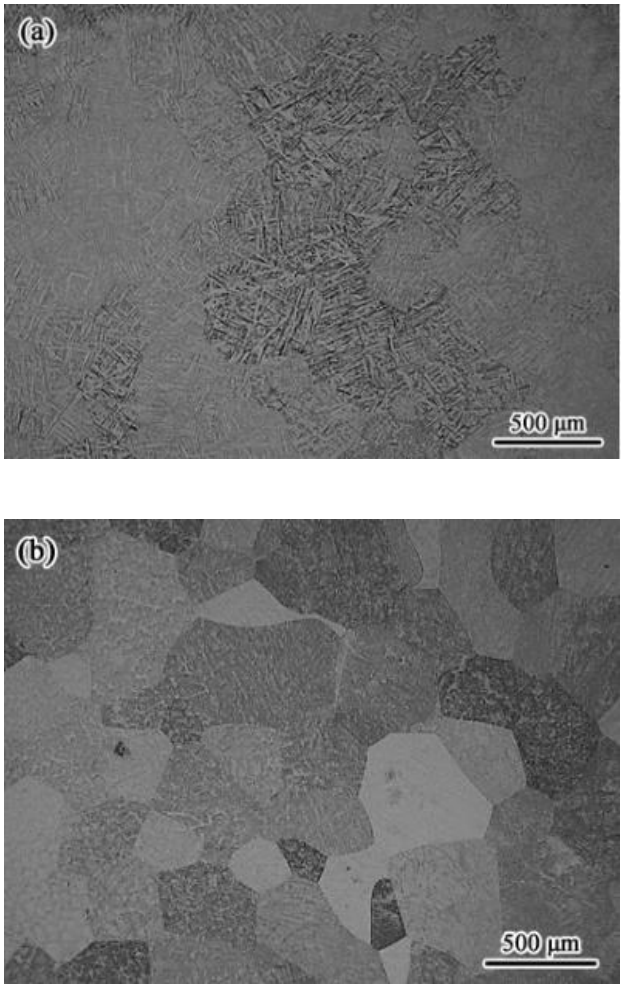

Figure 1 OM images of 12[Al-Ti12](AlTi2)+5[Al-Ti14](V2Ti) (a), and 4[Al-Ti12](AlTi2)+12[Al-Ti14](V2Ti)

Fig. 2 shows the engineering stress-strain curves of 12[Al-Ti_{12}]($AlTi_2$)+5[Al-Ti_{14}](V_2Ti), and 4[Al-Ti_{12}]($AlTi_2$)+12[Al-Ti_{14}](V_2Ti) at room temperature. The UTS and YS with the cluster ratio of 12:5 alloy is 925±3 MPa and 793±2 MPa , respectively, and the ductility is 5±1%. Compared to the cluster ratio of 12:5 alloy, the cluster ratio of 4:12 alloy has a significantly increase of strength and ductility.The UTS and YS are 1045±5 MPa and 819±2 MPa, respectively, and the ductility is 13±2%.

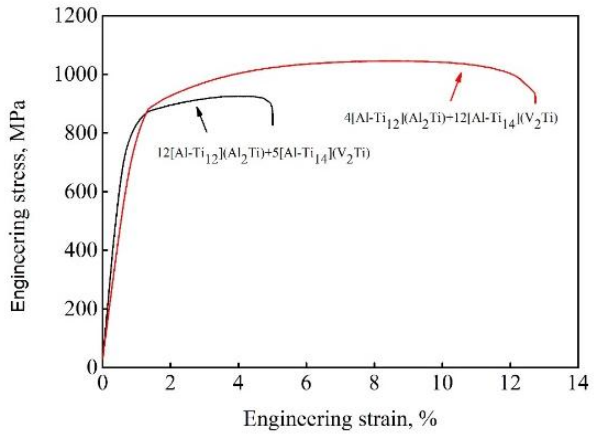

Figure 2 Engineering stress-strain curves at room temperature

4 Conclusion

Compared to Ti-6Al-4V, the tensile strength of Ti-4.13Al-9.36V alloy increased to 1045MPa, by 13%, and the ductility increased to 13.2%, by 164%.

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