

Microstructure and mechanical properties evolution of near- β alloy Ti-4Al-6Cr-5Mo-5Nb-xTa

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Abstract: In order to meet the current needs of the aerospace industry for aircraft with high thrust to weight ratio and lightweight in complex service environments, domestic fasteners with high specific strength and good plasticity have been developed for use β titanium alloys have become a current research hotspot. By calculating the Mo equivalent, the design belongs to the near- β alloy matrix composition within the titanium alloy range is Ti-4Al-6Cr-5Mo-5Nb, and the microstructure is controlled by adding alloy element Ta with a mass fraction of 0.4~2.0wt.%. Research has found that there is no new phase formation in the matrix, and as the Ta content increases, significantly more β phases, the β grain diameter decreased from 2.1 mm to 0.4 mm, the α phase tends to coarsen gradually. When adding 1.6 wt.% Ta, the tensile strength and fracture toughness reach the peak values of 735 MPa and 55 MPa $\cdot$ m^{1/2} respectively.

Keywords: Titanium alloy; Ta; Microstructure; Tensile strength; Fracture toughness

1. Introduction

High-performance near- β titanium alloys are critical structural materials in advanced aerospace and marine applications, driven by their exceptional strength-to-weight ratio^[1-3]. The development of next-generation components requires an exceptional synergy of mechanical properties, particularly high levels of both strength and fracture toughness^[4]. A fundamental challenge impeding this goal is the inherent strength-toughness trade-off, where conventional strengthening pathways often detrimentally affect fracture resistance^[5-7]. Therefore, innovative alloy design strategies are essential to overcome this antagonistic

relationship^[8,9].

Alloying with β -stabilizing elements is a proven approach to tailor the microstructure and mechanical properties of titanium alloys^[10,11]. Among these, Tantalum (Ta) is a particularly compelling candidate^[12]. As an isomorphous β -stabilizer, Ta effectively enhances the matrix strength via solid-solution strengthening^[13,14]. Crucially, its atomic radius is proximate to that of Ti, which minimizes lattice distortion and is thus beneficial for retaining toughness and ductility during strengthening^[15-18]. This assertion is supported by first-principles calculations, which indicate a strong interatomic bonding between Ta and Ti^[19], suggesting a

significant potential for improving mechanical performance^[20].

Our preliminary investigations identified the Ti-4Al-6Cr-5Mo-5Nb alloy as a promising castable system, yet it exhibits a suboptimal strength-toughness balance that fails to meet the stringent performance targets. To address this limitation, the present study systematically investigates the influence of micro-alloying with Ta on this base alloy. The primary objective is to achieve a concurrent enhancement in strength and toughness by strategically tailoring the microstructure, specifically through the refinement and morphological control of the α -phase precipitates. This work elucidates the governing mechanisms by examining the evolution of phase constitution, microstructural features, and the resultant mechanical properties in the newly developed Ti-4Al-6Cr-5Mo-5Nb- x Ta alloys.

2. Materials and methodology

Alloys with nominal compositions of Ti-7Mo-4Al-3Nb-2Cr-2Zr- x Ta ($x = 0, 0.4, 0.8, 1.2, 1.6$, and 2.0 wt.%) were prepared from high-purity starting materials. These included sponge Ti (≥ 99 wt.%), sponge Zr (≥ 99 wt.%), Mo, Al, Cr, Ta (≥ 99 wt.%), and a Ti-50Nb master alloy. The fabrication was conducted in a high-vacuum arc furnace, where each ingot was flipped and remelted four times to achieve a homogeneous distribution of the constituent elements.

The chemical compositions of the alloys were verified using an Axios-PW4400 X-ray Spectrometer. Phase identification was performed by X-ray diffraction (XRD) with a Cu $K\alpha$ radiation source. The phase transformation temperatures were determined via

differential scanning calorimetry (DSC). For microstructural characterization, a suite of microscopy techniques was employed, including optical microscopy (OM, Olympus GX71), scanning electron microscopy (SEM, Merlin Compact), and transmission electron microscopy (TEM, FEI Talos F200X).

Mechanical properties were evaluated at ambient temperature using an Instron5569 universal testing machine. Uniaxial tensile tests were performed on dog-bone shaped specimens with a gauge section of $15 \text{ mm} \times 2.2 \text{ mm} \times 2 \text{ mm}$ (length $\times$ width $\times$ thickness). For fracture toughness evaluation, single-edge notched specimens with dimensions of $16 \text{ mm} \times 4 \text{ mm} \times 2 \text{ mm}$ were utilized. The tests were conducted at constant crosshead speeds of 1 mm/min for tension and 0.5 mm/min for fracture toughness, respectively. To ensure statistical reliability, all reported values are the average of at least three independent tests.

3. Results

3.1 The chemical composition with different Ta content

The chemical composition of the prepared alloy was tested and the results are shown in Table 1. The results show that the actual chemical composition is similar to the nominal composition, and the content of impurity elements detected is small and negligible, therefore, it is considered that the alloy ingot obtained by vacuum cold crucible arc melting can meet the needs of the designed composition, and the prepared ingot can well reflect the microstructure and mechanical properties of the designed component, and the ingot melting has achieved good results.

Table 1 The nominal component and chemical composition of selected alloys (wt.%)

x Ta	Chemical composition					
	Ti	Al	Cr	Mo	Nb	Ta
0Ta	Bal.	3.92 ± 0.12	6.04 ± 0.06	4.91 ± 0.17	5.09 ± 0.09	-
0.4Ta	Bal.	4.05 ± 0.12	5.86 ± 0.06	4.88 ± 0.17	4.89 ± 0.09	0.42 ± 0.01
0.8Ta	Bal.	3.88 ± 0.12	5.93 ± 0.06	4.95 ± 0.17	5.07 ± 0.09	0.85 ± 0.01
1.2Ta	Bal.	3.81 ± 0.12	5.98 ± 0.06	4.99 ± 0.17	4.82 ± 0.09	1.17 ± 0.01
1.6Ta	Bal.	4.07 ± 0.12	6.01 ± 0.06	5.07 ± 0.17	4.99 ± 0.09	1.64 ± 0.01
2.0Ta	Bal.	4.01 ± 0.12	5.92 ± 0.06	5.01 ± 0.17	4.92 ± 0.09	2.02 ± 0.01

3.2 Phase content with different Ta content

The phase constitution of the as-cast Ti-4Al-6Cr-5Mo-5Nb- x Ta alloys was characterized by

X-ray diffraction (XRD), with the patterns presented in Fig. 1. The results indicate that all alloys are composed of a primary body-centered cubic (BCC) β phase and

trace amounts of a hexagonal close-packed (HCP) α phase. The absence of any additional peaks confirms the complete solid solution of Ta within the alloy matrix.

A key observation from the diffractograms is a systematic shift of all peaks toward higher 2θ angles with increasing Ta content. As detailed in Fig. 1(a), the prominent β -(110) peak shifts from 39.38° to 40.10° as Ta concentration increases from 0 to 2.0 wt.%. Similarly,

the α -(103) peak shifts from 70.16° to 71.32° (Fig. 1(b)). According to Bragg's Law, this shift to higher diffraction angles corresponds to a decrease in the interplanar spacing (d-spacing), signifying a contraction of the unit cell lattice. The low intensity of the α -phase reflections is characteristic of the as-cast, untransformed microstructure typical for this near- β alloy system.

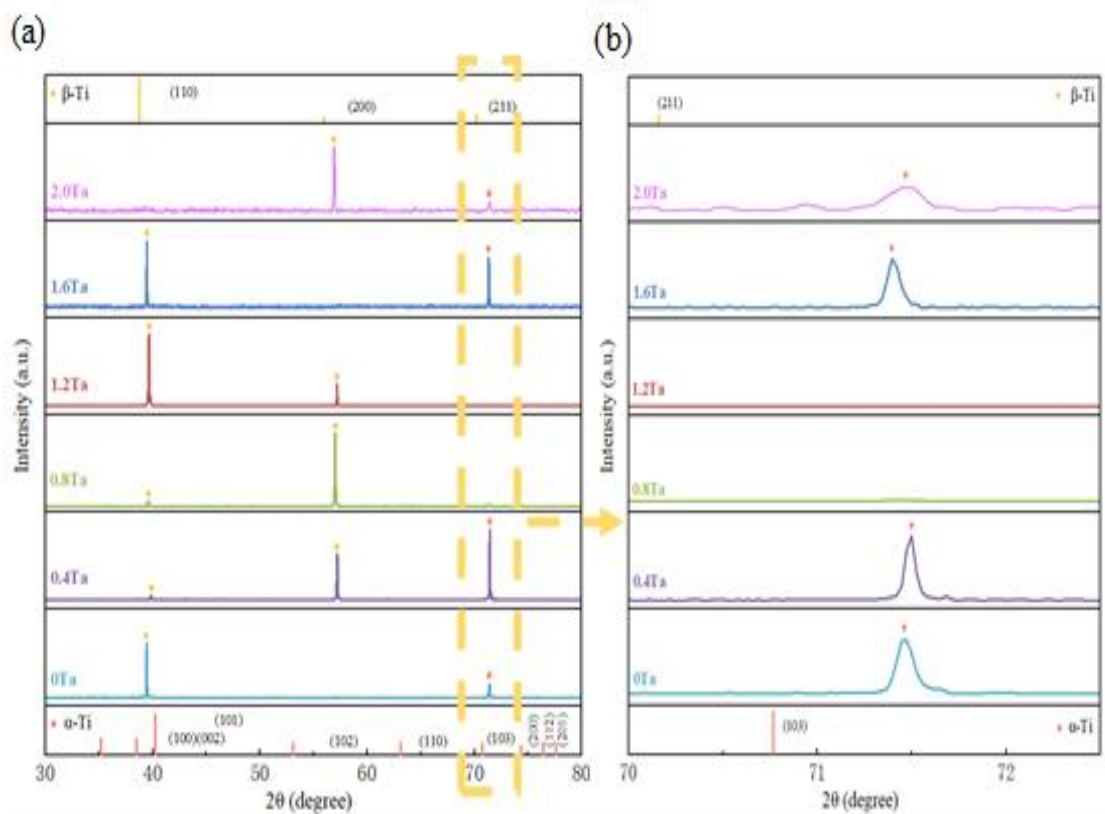


Fig. 1 XRD results of Ti-4Al-6Cr-5Mo-5Nb-xTa alloys: (a) XRD pattern, (b) the highlight of the Fig. 1 (a).

3.3 Phase transition temperature with different Ta content

The high-temperature DSC curve of the designed alloy Ti-4Al-6Cr-5Mo-5Nb-xTa is shown in Fig2. When the temperature of the alloys rises from room temperature to the upper temperature limit (1100°C), only a unique exothermic peak is observed for each alloy. Among them, the alloy with 0.4wt.%Ta added had the highest exothermic peak, about 780°C . As the Ta content increases to 2.0wt.%, the phase transition temperature from α -Ti to β -Ti decreases to 721°C . In addition, no significant endothermic peaks were observed during the cooling of the alloys of the five design components.

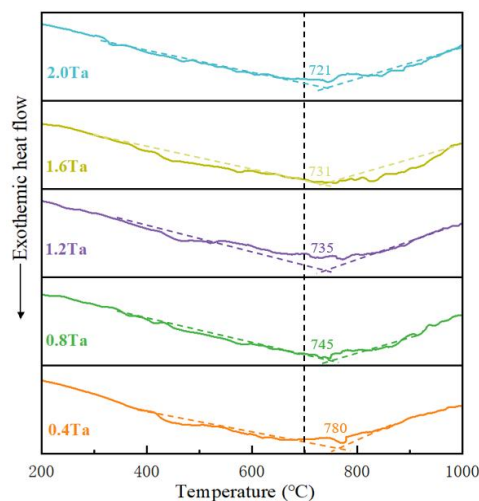


Fig.2 The DSC test results of Ti-4Al-6Cr-5Mo-5Nb-xTa alloys.

3.4 Microstructures and morphology of β grain with different Ta content

Fig.3 is the microstructure image of Ti-4Al-6Cr-5Mo-5Nb-xTa, observing the scanning image, it can be seen that the cast structure of the alloy is mainly dominated by β grains, and almost no α phase can be observed, which is because Ta element belongs to the isomorphous β stable element, which can effectively reduce the transition temperature of the $\beta \rightarrow \alpha$ phase. In

addition, Ta element and Nb element belong to the same family, can play the role of displacement solid solution, and have the same bcc crystal structure as β titanium alloy, so Ta element can be infinitely solid soluble in the β phase inside the alloy. At the same time, the solidification temperature range of Ta element is very narrow, and there is almost no segregation, so Ta element hardly forms a compound phase with Ti.

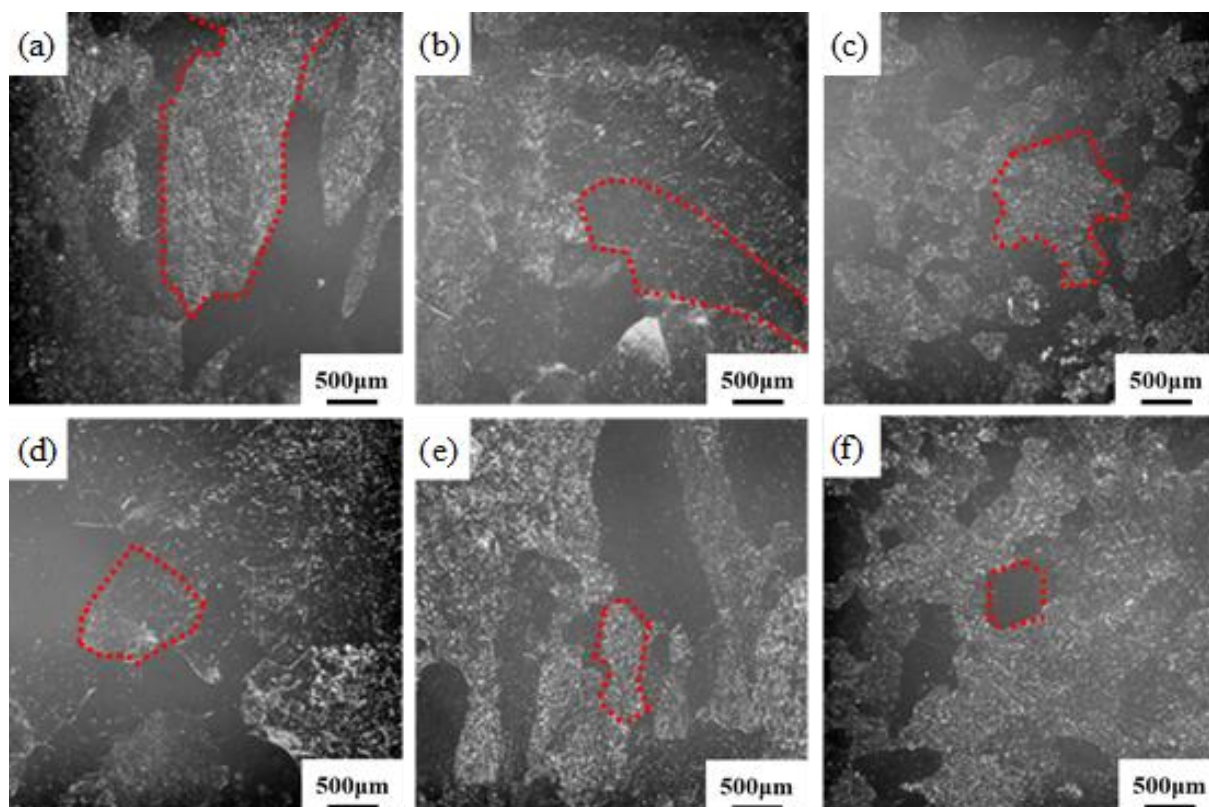


Fig.3 SEM images under the low magnification of Ti-4Al-6Cr-5Mo-5Nb-xTa alloys

(a) 0Ta; (b) 0.4Ta; (c) 0.8Ta; (d) 1.2 Ta; (e) 1.6Ta; (f) 2.0Ta.

It is worth noting that the β grains in the tissue change significantly with the change of the content of the added Ta element. From the perspective of morphology, with the continuous increase of the content of Ta element, the β grains gradually changed from slender columnar to equiaxed grains. At the same time, from the perspective of grain size, the size of β grain is constantly refined. In order to quantitatively calculate the average size of the grain, the microstructure of the alloy was collected by multi-region and multi-view scanning pictures, and the average size of the grain was counted and calculated by the equivalent circle diameter, and the image was drawn as shown in Fig.4. It was observed that the size of the β grain decreased from 2.4 mm to 0.3 mm, so as the content of Ta element increased from 0 to 2.0 wt.%, the grain size decreased by 87.5%.

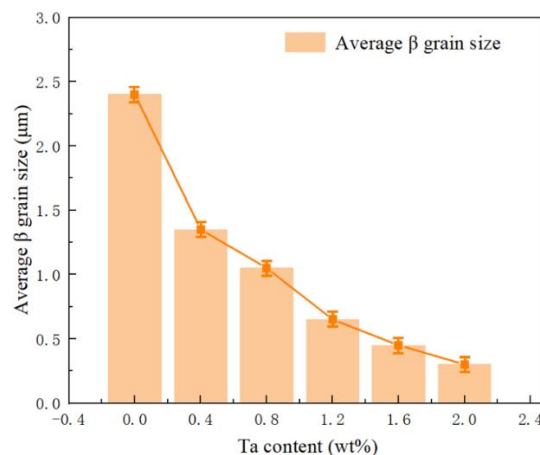


Fig.4 The average β grain size.

Fig.5 is an SEM image of the design alloy composition Ti-4Al-6Cr-5Mo-5Nb-xTa observed under a

high-magnification microscope, from which it can be seen that only α and β phases exist, which once again confirms that the Ta element can be infinitely soluble with β -Ti without other new phases. In addition, the cast structure of the alloy is coarse β grains and primary α phase (α_p) and secondary α phase (α_s) diffused in the matrix, in which the primary α phase presents an elongated band, while the secondary α phase is smaller granular. With the increase of Ta content, the β grain gradually changed from coarse columnar grain to small equiaxed grain, and the density of the α phase of the intragrain diffusion distribution increased. Observation in the crystal can also show that the size (length and width) of the primary α phase (α_p) shows a trend of increasing and then decreasing, and at the same time, the orientation of the α_p phase is also disorderly and gradually appears to a certain orientation, which improves the plasticity of the alloy to a certain extent. The large primary α phase (α_p) can also hinder crack propagation, change the crack

propagation path, increase the force required for crack propagation, and thus improve the fracture toughness of the alloy. The observation of the secondary α phase (α_s) showed that the size of the α_s phase was uniform, and the trend of increasing and decreasing with the increase of Ta content also showed a trend of increasing and decreasing. It is worth noting that with the addition of Ta element, the distribution of α phases at grain boundaries becomes more and more complete, and the size of the α phase peaks when the Ta content is 1.6wt.%. The dislocation motion at this point is more hindered at the grain boundaries, so the alloy has a high plasticity.

3.5 Tensile properties and fracture toughness with different Ta content

Tensile strength tests and fracture toughness tests were conducted and the values of ultimate tensile strength, yield tensile strength, elongation, and fracture toughness for the designed alloys are summarized in Table 2.

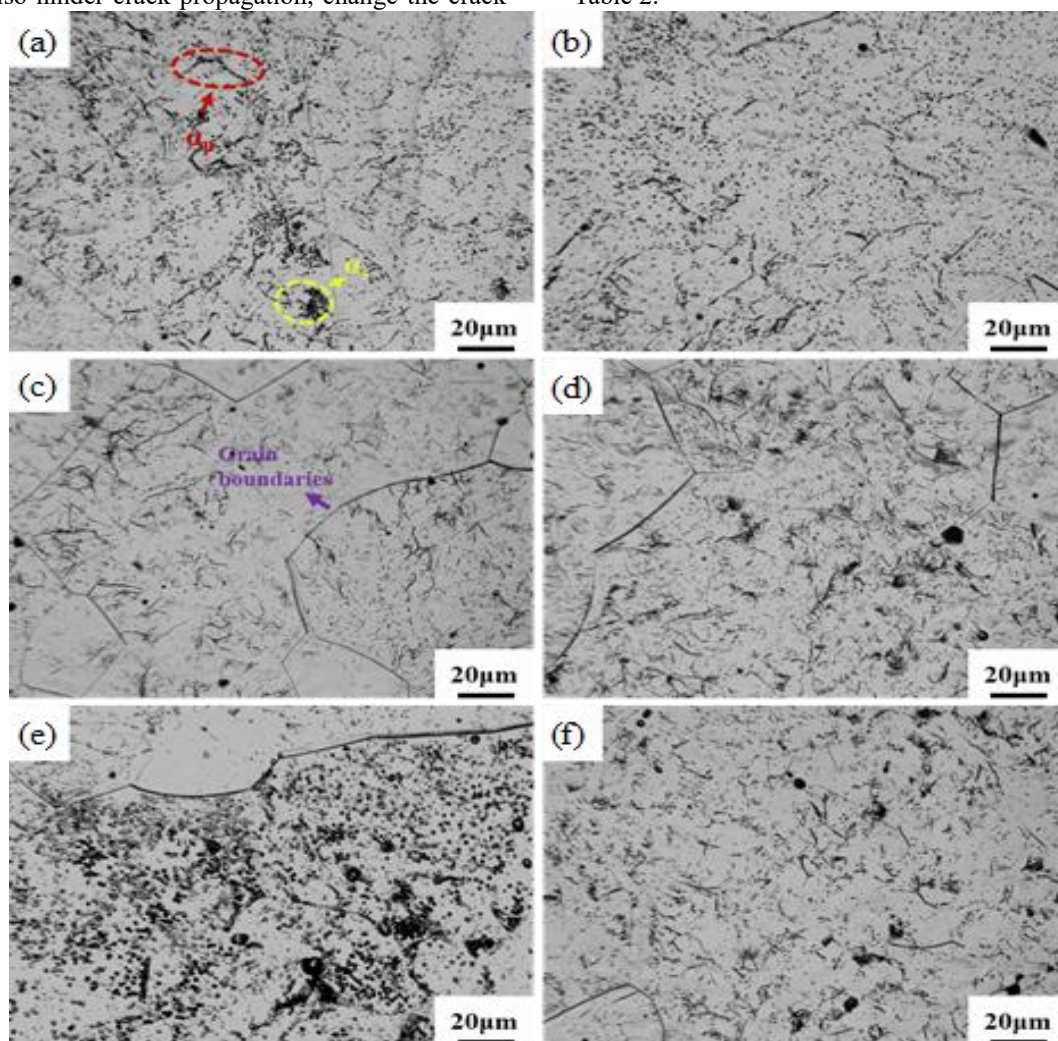


Fig.5 SEM images under the high magnification of Ti-4Al-6Cr-5Mo-5Nb-xTa alloys

(a) 0Ta;(b) 0.4Ta;(c) 0.8Ta;(d) 1.2 Ta;(e) 1.6Ta;(f) 2.0Ta.

Table 2 Tensile properties and fracture toughness of Ti-4Al-6Cr-5Mo-5Nb-xTa alloys.

Alloy	UST (MPa)	YST	EI (%)	K _{IC} (MPa·m ^{1/2})
0Ta	694±25	654±32	36.3±1.3	41±3
0.4Ta	707±28	668±42	38.1±1.4	45±4
0.8Ta	723±32	678±37	39.2±1.2	46±4
1.2Ta	725±21	682±29	40.1±1.3	50±2
1.6Ta	735±35	701±38	50.1±1.2	55±3
2.0Ta	729±26	699±24	44.6±1.4	49±3

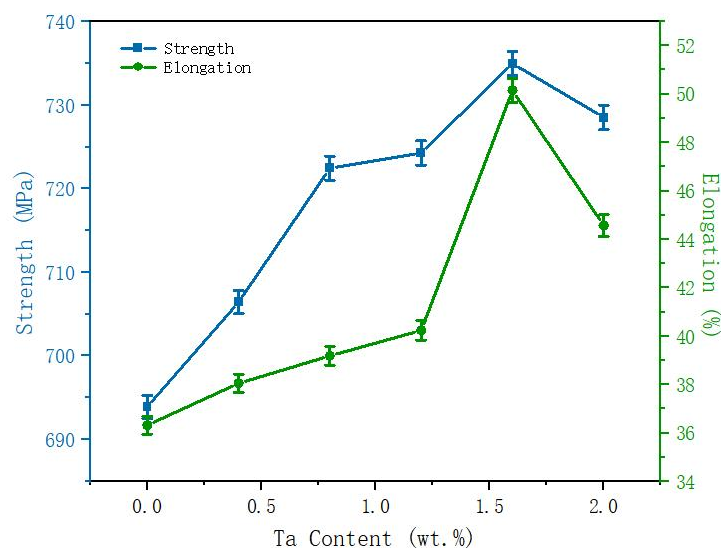


Fig.6 Tensile properties of Ti-7Mo-4Al-3Nb-2Cr-2Zr-xTa alloys for different Ta contents

Fig.6 depicts the relationship between the tensile properties of the designed alloy and the content of the added Ta element. The influence mechanism of Ta element content on the tensile strength of alloy is mainly due to the change of Ta content causing changes in the internal microstructure of the alloy. With the increase of Ta element content, the tensile strength of the alloy first increases and then decreases, which is similar to the change trend of elongation. The maximum tensile strength and elongation values of 0Ta alloy matrix are 694 MPa and 26.3%, respectively. When the Ta content increased to 1.6 wt.%, the tensile strength and elongation reached peak at 735 MPa and 50.1%, respectively. Compared with 0Ta alloy, the tensile strength and elongation are increased by 5.9% and 38.1%, respectively.

Fig.7 below shows the tensile fracture morphology of the designed alloy composition. As shown in Fig.7(a) and (a'), the fracture mode of the alloy matrix without element Ta is an obvious mixed fracture form, and there

are typical characteristics of brittle and ductile fracture. With the addition of Ta element, the characteristics of ductile fracture in the fracture morphology of the alloy began to dominate, and the fracture mechanism changed to a typical microporous aggregation fracture, indicating that the plasticity of the alloy was significantly improved. In addition, ligament sockets of different densities, phase interfaces, tearing edges and some river patterns can be observed in the fractures of all components. With the increase of Ta element content, the size of the tendon socket gradually increased, the large tendon socket increased, and when the Ta content reached 1.6wt.%, it reached the maximum value, indicating that the toughness increased to the peak at this time. When the Ta element is not added, there is an obvious tear edge in the fracture morphology, and with the addition of the Ta element, this feature begins to decrease and gradually disappear, and when the Ta content reaches 2.0wt.%, the tear edge reappears, as shown in Fig.5(f), indicating that excessive Ta element will deteriorate the plasticity of the alloy, which is also confirmed by the tensile strength

curve. At the same time, the interface of α/α and α/β phases can be observed in Figure.7(b) and (e), which on the one hand helps the propagation of cracks and improves the plasticity of the alloy, on the other hand, the

refined α_s phase may hinder the propagation of microcracks and promote the improvement of alloy strength.

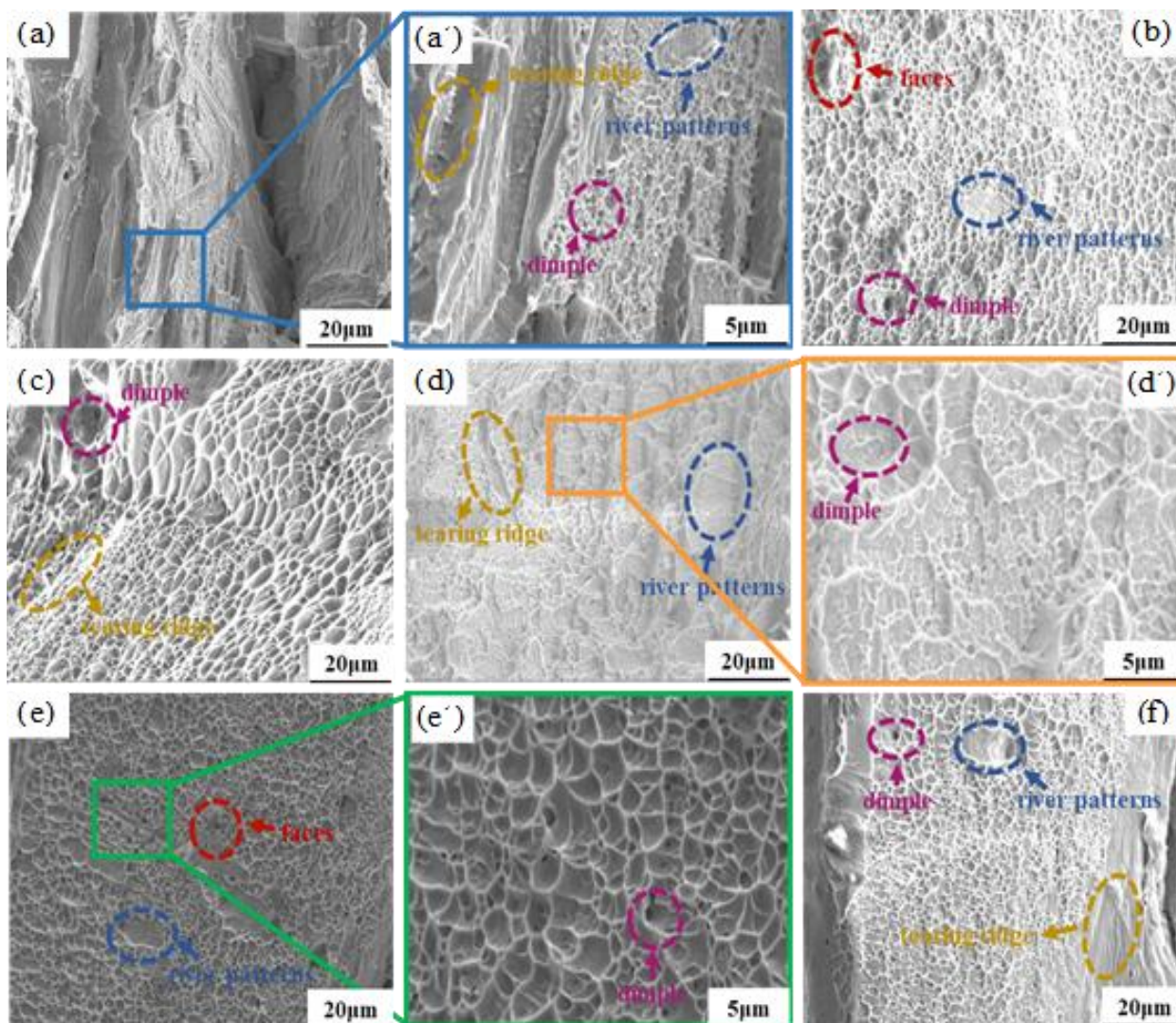


Fig.7 Fracture morphology and crack propagation pathways of Ti-7Mo-4Al-3Nb-2Cr-2Zr-xTa

(a)(a')0Ta;(b)0.4Ta;(c)0.8Ta;(d)(d')1.2Ta;(e)(e')1.6Ta;(f)2.0Ta

Fig.8 below shows the fracture toughness values of Ti-4Al-6Cr-5Mo-5Nb-xTa alloy with different contents of Ta elements, and it is observed that the fracture toughness number of the alloy increases first and then decreases with the increase of Ta. When the content of Ta element is 0wt.%, the collective fracture toughness value of the alloy is 41MPa·m^{1/2}, which is at a medium level in the nearly β titanium alloy in the cast state. When the content of Ta element added to the designed alloy Ti-4Al-6Cr-5Mo-5Nb reached 1.6wt.%, the fracture toughness of the alloy reached a peak of 55 MPa·m^{1/2}, which was 34.1% higher than that of 0Ta alloy. The increase of surface Ta content has a significant effect on the improvement of the fracture toughness of the alloy.

However, when the amount of Ta element added reaches 2.0wt.%, the fracture toughness of the alloy begins to decrease, and the reason for this phenomenon is that the over-refinement of the α phase will reduce the fracture toughness of the alloy. It is worth noting that with the addition of Ta element, the strength and toughness of the alloy have been significantly improved. Therefore, it is believed that Ta element has a good effect on the simultaneous enhancement of the strength and toughening of nearly β titanium alloys, and the subsequent heat treatment and thermal deformation of the designed Ti-4Al-6Cr-5Mo-5Nb-xTa alloy to achieve the goal of strengthening and toughening has high research value.

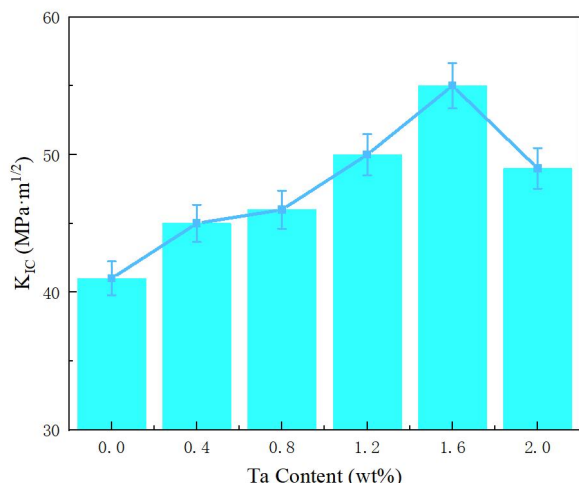


Fig.8 The values of fracture toughness of
Ti-4Al-6Cr-5Mo-5Nb-xTa

4. Discussion

4.1 The analysis of Ta effect on the phase content and size

As a common β stable element, Ta element will be solidly dissolved into the β phase of the alloy in the form of Nb element in the displacement collective, so the addition of Ta greatly enhances the stability of the β phase. In addition, as an element with high melting point, large atomic radius and slow diffusion rate, Ta will hinder the transition process from β phase to α phase in the matrix. Therefore, with the increase of Ta content in the alloy, the phase transition process from the β phase to the α phase becomes difficult, therefore, the α phase content in the alloy decreases and the content of the β phase increases. In addition, displacing the Ta element solidly dissolved in the matrix promotes nucleation as a solute atom and inhibits the growth rate. The increase in Ta content can also promote the nucleation of the α phase in more orientations, thereby reducing the size of the α phase. From the measurement results of the phase transition temperature, it can be seen that as the Ta content increases, the phase transition temperature of the alloy decreases. Therefore, the generated α phase has sufficient time to grow, and when the Ta content exceeds 1.6wt.%, it will lead to a slight increase in the size of the α phase.

4.2 The effect of Ta addition on β grain

As a high melting point alloying element, Ta promotes the heterogeneous nucleation of β grains, resulting in the competitive growth of β grains and resulting in the refinement of β grains. In addition, the increase in Ta content also causes the solidification front

to produce component supercooling. And to a certain extent, it can also increase the nucleation points in the liquid phase region, resulting in the refinement of β grains. The microstructure refinement effect of Ta on titanium alloys is also related to its influence on the parameters related to the crystallization process of the alloy [21]. When the new phase crystallizes in a melt that satisfies the supercoolance condition, its expression for the uniform nucleation rate N is shown in Equation(1):

$$N = K_v \exp(-\Delta G_k/kT) \exp(-\Delta G_A/kT) \quad (1)$$

where K_v refers a constant, ΔG_k stands for the nucleation energy, ΔG_A represents the activation energy of atoms transferred from liquid to nucleus. The nucleation energy of new phase, ΔG_k , is described as follows:

$$\Delta G_k = \frac{16\pi\sigma^3 T_m}{3(L_m \cdot \Delta T)^2} \quad (2)$$

Ta reduces the interfacial energy σ as a surface active substance. Thus, the nucleation energy ΔG_k is reduced and the nucleation rate N is greatly improved.

4.3 Analysis on strength-toughness synergy mechanism of Ti-4Al-6Cr-5Mo-5Nb-xTa alloys

It can be seen from Fig. 3-4 and Fig.6 that the tensile strength and fracture toughness of the designed alloy components show a trend of first increasing and then decreasing with the increase of the content of Ta element, and this synchronous increase of strength and toughness may be related to the displacement solution of Ta element in the matrix, the refinement of β grains, and the increase of grain boundaries.

Ta element is a typical β stable element, solid soluble in the matrix will show a crystal structure close to β -Ti. Therefore, the addition of element Ta to the near- β titanium alloy can play a good solution strengthening effect. When an appropriate amount of Ta is added, it can form a stable solid solution with β -Ti, so that the crystal structure of Ti has a certain lattice distortion. This distortion creates internal stresses inside the alloy that impede the slippage and climbing of dislocations. This promotes an increase in the tensile strength of the alloy, an effect that can be estimated using the dislocation-solute elastic interaction equation [22], as shown in Equation (3).

$$\sigma_{SS} = \left(\sum_i B_i^2 X_i \right)^{2/3} \quad (3)$$

On the other hand, the size of β grains varies with the increase of Ta content. The smaller the grain size, the greater the number of grain boundaries. As one of the strengthening methods, the role of grain boundary

strengthening cannot be ignored. The more grain boundaries, the greater the impediment to dislocations and the better the reinforcement. σ_{GB} is usually calculated by the classical Hall-Petch equation, which is proposed on the basis of the dislocation blocking model [23] in the form shown in Equation (4):

$$\sigma_{GB} = \frac{k}{\sqrt{d}} \quad (4)$$

where σ_{GB} stands the grain boundary strengthening, the k value for the Ti alloy substrate is $750 \text{ MPa} \cdot \mu\text{m}^{1/2}$ [24].

5. Conclusions

This chapter mainly analyzes and tests the casting microstructure, phase composition, tensile strength and fracture toughness of the design component Ti-4Al-6Cr-5Mo-5Nb-xTa, explores the effect of the addition of element Ta on the properties of the alloy, and screens the components of the subsequent thermal flux, and the main conclusions are as follows:

(1) When the content of Ta element increased from 0 to 2.0wt.%, no new phase was formed in the tissue, Ta element was almost completely dissolved in the β phase, and the content of the β phase increased, and the size of the α phase first increased and then decreased.

(2) When the content of Ta element increased from 0 to 2.0 wt.%, the β grain diameter decreased from 2.1 mm to 0.4 mm. Ta's large atomic radius hinders the growth of β grains, thereby limiting the transition from the β phase to the α phase.

(3) When the content of Ta element increased from 0 to 1.6wt.%, the tensile strength and fracture toughness increased simultaneously, from 694 MPa and 41 $\text{MPa} \cdot \text{m}^{1/2}$ to 735 MPa and 55 $\text{MPa} \cdot \text{m}^{1/2}$, respectively. When the Ta content exceeded 1.6wt.%, the strength and toughness decreased.

(4) When the content of Ta element increases from 0 to 2.0wt.%, on the one hand, it can replace the Nb element in the matrix, causing lattice distortion, thereby playing the role of solid solution strengthening, on the other hand, Ta, as a heteromorphic nucleus point, will promote the refinement of β grain grains and increase the number of grain boundaries in the tissue, thereby playing the role of grain boundary strengthening.

(5) Ti-4Al-6Cr-5Mo-5Nb-1.6Ta has the highest tensile strength and fracture toughness, so this component was selected for subsequent thermal deformation simulation experiments.

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