

Study on the Microstructure and Properties of Cast High-Temperature Titanium Alloy Based On Cluster Model Design

Tianyu Liu ^{1,*}, Xinqi Li ¹, Weichen Qiu ¹, Hongyu Liu ¹, Hongyu Liu ¹, Shibing Liu ¹, Kun Shi ¹

¹ National Key Laboratory of Advanced Casting Technologies, China Academy of Machinery Shenyang Research Institute of Foundry Co., Ltd. Shenyang 110022, China

*Corresponding address: e-mail: liutianysrif@163.com.com

Abstract: High-temperature titanium alloys have the characteristics of light weight, high strength and high temperature resistance, and are widely used in compressor discs, blades and casing of aeroengines. With the further improvement of aero-engine performance, the service temperature of high-temperature titanium alloys parts is increasing, and it is urgent to develop novel high-temperature titanium alloy with resistance above 600°C. In this paper, we designed a series of high-temperature titanium alloys based on the cluster-plus-glue-atom model which describe the short-range order, and studied the influence of alloy elements Mo, Nb, Ta and W on the microstructure, mechanical properties and casting properties of cast high-temperature titanium alloys by OM, SEM, tensile and spiral test methods. The results show that with the increase of [Mo]_{eq}, the alloy strength increases at room temperature, but the alloy strength gradually decreases at 650 °C. Among the four alloy elements of Mo, Nb, Ta and W, the increase of Mo content significantly broadens the solidification range of the alloy, resulting in the greatest influence of Mo on the fluidity of high-temperature titanium alloys, followed by Ta, Nb and W.

Keywords: cast; high-temperature titanium alloy; composition design; the cluster-plus-glue-atom model

1 Introduction

Titanium alloys are widely used due to their good properties in strength, toughness, formability, weld-ability, corrosion resistance and biocompatibility [1]. However, the solid solution strengthening and aging precipitation strengthening that existing high-temperature titanium alloys rely on will reach their limit at 600°C, and further increasing the temperature of the alloy will make it difficult to meet the requirements of thermal strength indicators. At present, high-temperature titanium alloys are mainly characterized by "Ti-Al-Sn-Zr-Mo-Si" multi-component solid solution strengthening. By optimizing the alloy elements and composition, it is still possible to further improve the high-temperature performance of the alloy [2]. In our preliminary work, Mo, Nb, Ta, W, and Si occupied the positions of β-phase cluster type connecting atoms, Sn occupied the positions of α-phase cluster type connecting atoms, Al occupied the positions of α-phase cluster type center and connecting atoms, as well as the positions of β-

phase cluster type center atoms, and Zr occupied the shell positions of both α- and β-phase cluster types [3]. This article is based on the cluster and connected atom model, and obtains the composition of high-performance cast high-temperature titanium alloy by regulating the matching relationship of alloy elements.

2 Experiment Procedure

In the preliminary work, based on the α and β phase compositions of Ti-6Al-4V alloy, we determined the ideal cluster structural units and their ratios for the two phases, namely α - [Al-Ti₁₂] (AlTi₂): β - [Al-Ti₁₄] (V₂Ti) ≈ 2.34:1, where the square and small brackets represent clusters and connecting atoms, respectively. Then, the two structural units are regarded as two hard spheres with different radii, and a hard sphere stacking model is constructed. Analogous to atomic resonance theory, it is calculated that one stacking unit contains 17 hard spheres, and the ratio of the two structural units is uniquely determined to be 12:5. Therefore, the cluster structure of Ti-6Al-4V alloy is α-[Al-Ti₁₂](AlTi₂): β-[Al-Ti₁₄](V₂Ti), and the ideal alloy composition is Al_{10.28}V_{3.55}Ti_{86.18} (at.%)=Ti-6.05Al-3.94V (wt.%) [4].

The basic cluster structure of the alloy designed in this article is 12 [Al-Ti_{11.5}Zr_{0.5}] (Al_{1.25}Sn_{0.25}Ti_{11.5})+5 [Al_{0.8}Si_{0.2}Ti_{13.2}Zr_{0.8}] (MoNbTaWTi)₃. Using the cluster structure as a limiting condition, a joint orthogonal experiment was conducted to investigate the effects of alloying elements Mo, Nb, Ta, and W on the microstructure, mechanical properties, and casting performance of high-temperature titanium alloys.

Table 1 Design of alloy composition based on the cluster formula of 5 [Al_{0.8}Si_{0.2}Ti_{13.2}Zr_{0.8}] (MoNbTaWTi)₃

number	Mo	Nb	Ta	W
1	0.2	0.2	0	0
9	1	1	0.2	0

3 Mechanical properties of designed titanium alloys

Figures 1 shows the metallographic structures of alloys 1# and 9# after HIP, respectively. As shown in the figure, the microstructures of both alloys are composed of β-equiaxed crystals, with a Weibull structure within the β-crystals.

(a)

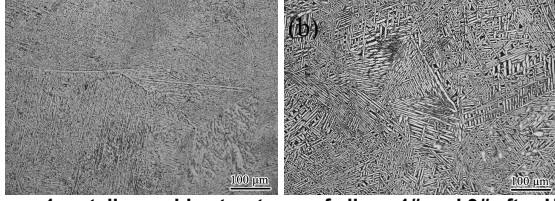
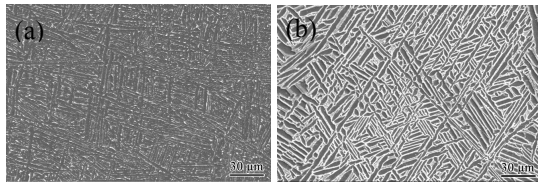


Figure 1 metallographic structures of alloys 1# and 9# after HIP:
(a)1#; (b)2#

Figures 2 shows the SEM of 1# and 9# alloys after HIP, respectively. It can be seen from the figure that the β equiaxed crystal of 1# alloy is composed of acicular α phase, and the β equiaxed crystal of 9# alloy is composed of lath α phase. Compared to alloy 1#, alloy 9# exhibits a significant coarsening of the alpha phase.



Figures 2 The SEM of 1# and 9# alloys after HIP:
(a)1#; (b)2#

According to the formula of Bania's $[Mo]_{eq}$ ^[5], The stability ability of the β -phase is Mo, W, Nb, and Ta in sequence. Furthermore, according to Bania's $[Mo]_{eq}$ formula, the $[Mo]_{eq}$ of alloy 1# is -5.26, and the $[Mo]_{eq}$ of alloy 9# is -1.32.

Table 2 shows Mechanical properties of different alloy composition at room temperature and 650°C. As shown in the table, with the increase of $[Mo]_{eq}$, the strength of the alloy increases in room temperature but decrease in 650°C. The elongation rate is on the contrary.. This is because with the increase of $[Mo]_{eq}$, the stability ability of the alloy's β -phase is enhanced, that is, the content of β phase in the alloy increases, resulting in an increase in the interface between α - and β -phases, which is conducive to hindering dislocation movement, thereby improving the strength of the alloy and reducing its elongation. However, as shown in

Figure 4, the alpha phase of alloy 9# is significantly coarsened. This is beneficial for improving the average free path of dislocation movement and increasing the elongation of the alloy.

Table 2 Mechanical properties of different alloy composition at room temperature and 650°C

temperature	number	Rm/MPa	R _{p0.2} /MPa	A/%
room	1#	958±2	843±1	10±1
	9#	1004±2	888±2	9±2
650°C	1#	582±2	419±3	5.6±1
	9#	537±1	307±2	12.5±1

4 Conclusion

After HIP, compared to the intragranular α -phase of alloy 1#, the α -phase of alloy 9# significantly coarsens;

At room temperature, as $[Mo]_{eq}$ increases, the alloy strength increases; At 650 °C, as $[Mo]_{eq}$ increases, the alloy strength gradually decreases;

Acknowledgments

This work was supported financially by the Natural Science Foundation of Shenyang, China (Grant No. 22315605).

References

- [1] Banerje, D., Williams, J. C. Acta Mater, 61, 2013, 844-879.
- [2] YUE K, LIU J, ZHU S, et al. Origins of different tensile behaviors induced by cooling rate in a near alpha titanium alloy Ti65[J]. Materialia, 2018, 1: 128-138..
- [3] LIU T Y, LOU Y C, ZHANG S, et al. A novel Ti-5.55Al-6.70Zr-1.50V-0.70Mo-3.41Nb-0.21Si alloy designed using cluster-plus-glue-atom model for laser additive manufacturing[J]. China Foundry, 2023, 20(5): 414-422.
- [4] LIU T Y, ZHANG S, WANG Q, et al. Composition formulas of Ti alloys derived by interpreting Ti-6Al-4V[J]. Science China Technological Sciences, 2021, 64: 1732-1740.
- [5] MEHJABEEN A, XU W, QIU D, et al. Redefining the β -Phase Stability in Ti-Nb-Zr Alloys for Alloy Design and Microstructural Prediction[J]. JOM, 2018, 70(10): 1-6.