The Role of Minor Oxygen on Tensile Propertiesin Cast Ti-6Al-4V Alloy

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Abstract: In this paper, the effect of oxygen content in the range of 0.15 ~ 0.44 wt.% on the mechanical properties at room temperature of cast Ti-6Al-4V alloy was studied, and the mechanism of oxygen effect on its tensile deformation behavior was discussed. The results show that with the increasing of oxygen content, the strength of the alloy increases,while the elongation increases first and then decreases.It is found that oxygen solution in α-Ti leads to obvious change of lattice parameter c/aratio.The activation of prismatic slip of α-Ti will bring oxygen atoms from octahedral site to hexahedral site to reduce stacking fault energy. The reason why the strength of cast Ti-6Al-4V alloy increases and the ductility decreases with the increasing of oxygen content is that the lattice distortion caused by the solid solution of oxygen inα-Ti prevents the dislocation motion, while the abnormal ductility increasing at 0.22 wt.% oxygen content is due to the dislocation shuffling oxygen atoms into the hexahedral site.

Keywords: Cast Ti-6Al-4V Alloy,Oxygen Content, Mechanical Properties, Deformation Mechanism.

1 Introduction

Ti-6Al-4V alloy has good comprehensivemechanical properties and casting performance, is the most widely used cast (α + β) two-phase titanium alloy[1], oxygen is generally as interstitial atoms into theα-Ti lattice[2], play a hindering role to dislocation motion, with solid solution strengthening effect[3].But the mechanism by which the oxygen affects the mechanical properties is still lack of complete understanding. For this reason, this paper investigates the effect of oxygen content on the mechanical properties of Ti-6Al-4V alloy, and explores the essential mechanism of the effect of oxygen on the tensile properties of cast Ti-6Al-4Valloys.

2 Experimental procedure

In order to study how oxygen affected the mechanical properties of Ti-6Al-4V alloy, by changing the proportion of TiO_2 powder in the raw materials, 16mm Ti-6Al-4V casting rods with four oxygen contents were cast by cold crucible suspension smelting equipment, and then were subjected to hot isostatic pressing (HIP) at 920℃/130MPa/3h, named 0.15O, 0.22O, 0.26O and 0.44O respectively, according to the measured oxygen content of 0.15 wt.%, 0.22 wt.%, 0.26 wt.% and 0.44 wt.% . Tensile mechanical properties at room temperature were tested on an electronic universal material testing machine with a tensile rate of 0.45mm/min. The lattice constants of the samples were determined by selected area electron diffraction (SAED) using FEI TALOS F200X transmission electron microscope. Calculation result was based on the calculation principles of density functional theory and usedthe Vienna Ab initio Simulation Package (VASP) for calculations. The exchange correlation energy was represented by the PBE correlation functional potential in the generalized gradient approximation (GGA).

3 Result and discussion

Effect of oxygen on mechanical properties

Fig. 1(a) shows the stress-strain relationships of Ti-6Al-4V alloys with four oxygen contents at room temperature. It can be seen that there is almost no difference in yield and hardening conditions, which indicates that oxygen does not change its deformation mechanism in essence.

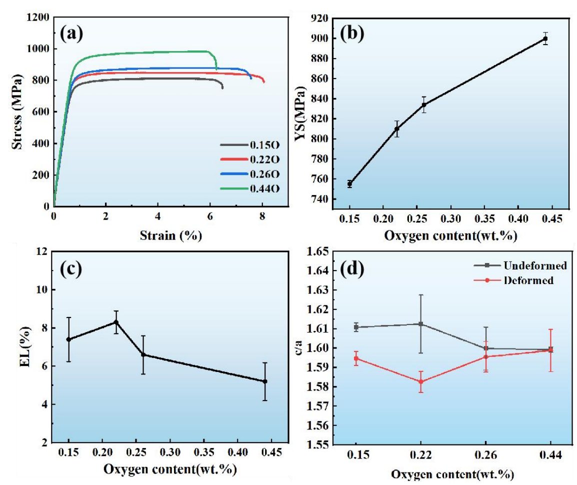

Fig. 1(a) Stress-strain relationships of Ti-6Al-4V alloys with four oxygen contents; (b, c) Changes of average yield strength and elongation with oxygen content; (d) The c/a ratio of the α phase before and after tensile deformation

Fig. 1(b) and (c) show the changes of average yield strength and elongation with oxygen content. With the increasing of oxygen content, thestrength of the alloys are linearly and positively correlated with oxygen content, which is obviously attributed to solution strengthening. The elongation decreases with the increasing of oxygen content, but the linear correlation is not big. It can be seen that the elongation does not decrease in accordance with the law in the range of 0.15 ~ 0.22 wt.% oxygen content, but increases slightly. This is different from the effect of single solution strengthening mechanism, so there must be another mechanism on ductility besides solution strengthening.We calculate the c/a ratio of theα phase before and after deformation by analyzingselected area electron diffraction,in Fig. 1(d).It can be seen that the c/a ratio of the α phase after deformation is smaller than before, and the decreasing degree is positively related to the ductility. It is speculated that the change of c/a ratio is related to the change of oxygen atom position during deformation and acts on ductility.

The role of oxygen in deformation mechanism

Interstitial energies at different sites of solid solution of oxygen in titanium were calculated by first-principles calculation through formula (1).The results are shown in Table 1. When oxygen is at octahedral site, the energy is the lowest, which is the most stable occupying site for oxygen.Energy of oxygen in hexahedral site is greater than that in octahedral site, which means that the hexahedral site is metastable occupying site.By relaxingthe α-Ti unit cells without oxygen and with oxygen at octahedral and hexahedral sites respectively, we find that oxygen increases the c/a ratioat octahedral site and decreases the c/a ratio at hexahedral site.

$$E_I = E_{Ti+O} - E_{Ti} - E_O \quad (1)$$

Table 1. Interstitial energy of oxygen in α-Ti

Position of oxygen	octahedral site	hexahedral site
Interstitial energy/eV	-8.85061	-7.6163

The prism plane of the α-Ti unit cells without oxygen and with oxygen at octahedral and hexahedral site is cut and the vacuum layer is established, and the slip is carried out with $\frac{1}{3}[11\bar{2}0]$ as Berger vector as shown in Figure 2(a). Through first-principles calculation, the stacking fault energy of prismatic slip is calculated at five points in a complete slip. The relationship between stacking fault energy and slip displacement is drawn in Fig. 2(b). It can be seen that the stacking fault energy of prismatic slip increases when oxygen at the stable octahedral site and decreases when oxygen at the metastable hexahedral site. Oxygen mainly occupies the octahedral site before deformation. The c/a ratio should increase gradually with the oxygen content, but the internal stress produced in casting and hot isostatic pressing produces a small number of dislocations in α phase,which shuffle oxygen from stable octahedral site to metastable hexahedral site with lower prismatic slip stacking fault energy. So that c/a ratio does not increase strictly with that increasing of oxygen content. After the deformation began, a large number of dislocations were produced in the lattice. Oxygen atoms were shuffled to hexahedral site, c/a ratio decreases.

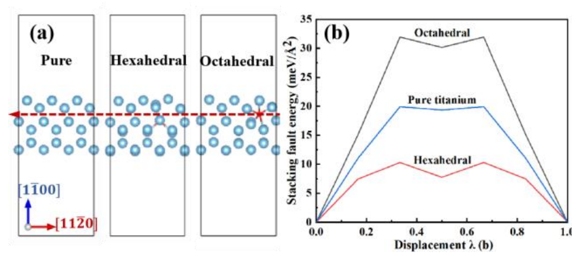

Fig. 2(a) prismatic slip of hexagonal α-Ti unit cells, without oxygen and with oxygen in hexahedral site and octahedral site; (b) The relationship between stacking fault energy and slip displacement.

The prismatic slip stacking fault energy decreases, the ductility problem caused by solid solution strengthening is alleviated.However, with the increasing of solid solubility of oxygen, the lattice distortion becomes larger, which hinders the dislocation activation and the dislocation shuffling oxygen atoms into the hexahedralsite. The c/a ratio decreasing degree decreases, and the ductility alleviation is inhibited.

Conclusion

The activation of prismatic slip shuffles theoxygen atoms from the octahedral to the hexahedral sites in order to reduce the stacking fault energy, exhibiting a decrease in c/a ratio and an alleviation of the damage to ductility.

Acknowledgments

This project was financially supported by Shaanxi Provincial Innovation Capacity Support Plan (2023-CX-TD-4), the State Key Laboratory of Solidification Processing(SKLSP202201) and ND Basic Research Funds, NPU (G2022WD).

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