Materials Characterization 139 (2018) 421–427

Contents lists available at ScienceDirect

Materials Characterization

journal homepage: www.elsevier.com/locate/matchar

Fabrication and characterization of a novel β metastable Ti-Mo-Zr alloy with large ductility and improved yield strength

JinYong Zhang[a,b,c,*], JinShan Li[b,**], GuanFang Chen[a], Lin Liu[c], Zheng Chen[a], QingKun Meng[a], BaoLong Shen[a], Fan Sun[d,**], Frédéric Prima[d]

[a] School of Material Science and Engineering, China University of Mining and Technology, Xuzhou, Jiangsu 221008, People's Republic of China
[b] State Key Laboratory of Solidification Processing, Northwestern Polytechnical University, Xi'an, Shaanxi 710072, People's Republic of China
[c] State Key Laboratory of Materials Processing and Die & Mould Technology, Huazhong University of Science and Technology, Wuhan, Hubei 430074, People's Republic of China
[d] PSL Research University, Chimie ParisTech-CNRS, Institut de Recherche de Chimie Paris, 75005 Paris, France

ARTICLE INFO

Keywords:
Alloy design
β-metastable titanium alloys
TRIP/TWIP effects
Mechanical behaviour
Microstructure
Deformation mechanism

ABSTRACT

In this paper, a novel ternary β-metastable titanium alloy, Ti-12Mo-5Zr (wt%), was designed based on the "*d*-electron" alloy design theory. The Ti-12Mo-5Zr alloy displays excellent combination of improved yielding stress (> 650 MPa), high ductility (uniform elongation ≈30%) and work-hardening behaviour. The detailed microstructural analysis indicates that the superior performances arise from the synergic effects between phase transformation induced plasticity (TRIP) and twinning induced plasticity (TWIP). Conforming to the design strategy, the improvement of mechanical performance results from the addition of Zr alloying element in substituting Ti, attributing to solution hardening effect and the increasing of critical resolved shear stress (CRSS) of stress induced martensitic transformation (SIM α″).

1. Introduction

Over the last few decades, titanium and its alloys have been attractive materials for aerospace, biomedical and sporting goods industries and automotive applications due to their high strength-to-density ratio [1,2], good hardenability [3,4], excellent fatigue/crack-propagation behaviour [5] and good corrosion resistance [1,6]. However, both their low ductility (total elongation typically < 0.25) and the lack of work-hardening compared with steels or Co-Cr alloys [1,7], limit the potential advanced applications where superior combination of strength and ductility are required. As a consequence, it is necessary to develop new Ti-alloys with combination of high strength, large ductility and a high work-hardening rate. More recently, a design strategy based on the semi-empirical "*d*-electron" alloy design theory has been proposed for titanium alloys to overcome these limitations [8,9]. The aim of design strategy is to activate a combined deformation mechanism involved in simultaneous mechanical twinning and phase transformations during plastic deformation. A new β-metastable Ti-alloy, namely Ti-12Mo (wt%) [8,10], has been designed for ductility improvement with large work-hardening behaviour, based on the semi-empirical "*d*-electron" alloy design theory. The experimental results [8,10] show that the Ti-12Mo alloy displays a superior combination of high strength, large ductility and high work-hardening rate, due to the simultaneous occurrence of Transformation Induced Plasticity (TRIP effects), Twinning-induced plasticity (TWIP effects) and dislocations slip [8–11]. In order to expand the family of the β-metastable titanium alloys with combined TRIP and TWIP effects, new ternary alloys are being elaborated through adding third alloying elements based on the design route of Ti-12Mo alloy. It has been proved that a substitution of Mo by other beta-stabilizers, e.x. in the newly designed Ti-9Mo-6 W [9], was able to maintain the TRIP/TWIP effects by design, and exhibiting better performance than the Ti-12Mo alloy. Alternatively, using neutral elements in the substitution strategy has been considered to be advantageous in fine-tuning of beta phase stability for strength improvement, according to our previous studies on superelastic alloys [12].

The Zr element was considered as neutral element since it has (nearly) no influence on the α/β phase boundary [13]. However, the Zr element in beta solid solution has been shown to decrease the martensitic start temperature (Ms) and retard ω phase formation [14]. Recent studies [12,15,16] have demonstrated that Zr is not neutral to phase transformation. Since Zr can affect the phase stability, it is reasonable to expect that Zr plays a role in the deformation mechanism as

* Correspondence to: J.Y. Zhang, School of Material Science and Engineering, China University of Mining and Technology, Xuzhou, Jiangsu 221008, People's Republic of China.
** Corresponding authors.
E-mail addresses: jyzhang@cumt.edu.cn (J. Zhang), ljsh@nwpu.edu.cn (J. Li), sun@chimieparistech.psl.eu (F. Sun).

https://doi.org/10.1016/j.matchar.2018.03.031
Received 24 September 2017; Received in revised form 13 March 2018; Accepted 21 March 2018
Available online 22 March 2018
1044-5803/

well. In this sense, Zr is no longer the neutral element, but work as the β-stabilizing elements in these metastable β-type Ti-alloys. In this paper, we designed a ternary Ti-12Mo-5Zr (wt%) alloy by mainly replacing Ti with Zr addition, keeping the same content of the Mo element. We aim to study the fact whether Zr addition also shows similar effectiveness in the improvement of mechanical performance by a different path of substituting Ti by Zr element. The mechanical performances of the ternary alloy were investigated and microstructural characterizations were conducted by using X-ray diffraction (XRD), scanning electron microscopy (SEM) and transmission electron microscopy (TEM) techniques. Based on the detailed microstructural investigations, the deformation mechanisms underlying the mechanical behaviour are discussed to clarify the validation of the design strategy.

2. Experimental Procedures

2.1. Alloy Design

In this work, the chemical formulation of the Ti-Mo-Zr alloy was performed by "*d*-electron" alloy design theory. The design theory, developed by Morinaga [17], although initially built for elasticity engineering, is also instructive in predicting plastic behaviours due to its basic concept in establishing a physical background on phase stability. The nature of alloying development of the alloys can be generalized by using electronic configurations of the alloying elements as Bo and Md parameters. These two parameters can be calculated theoretically in bcc Ti using the DV–Xa molecular orbital method [17,18]. Bo, the bond order, measures the covalent bond strength between Ti and one alloying element. Md, the metal d-orbital energy of alloying transition-metal, quantifies the level of the electronegativity and the metallic radius of elements. From the starting point of pure Ti, average Bo and Md values ($\overline{Bo}$, $\overline{Md}$) can be calculated for each alloy. By plotting the two parameters, the alloy position is coordinated on the $\overline{Bo} - \overline{Md}$ map according to the alloy composition. Moreover, this map also allows drawing "alloying vectors" for binary alloys Ti-M (M = alloying element). The "alloying vector" of alloying elements represents their characteristics in stabilizing the binary alloys. With these parameters, the phase stability and the deformation mechanism can be predicted by reaching certain area of interests on the $\overline{Bo}$–$\overline{Md}$ map. This map is of great interest because it can be used as a tool to predict "as-quenched" properties of titanium alloys, independently from the number of alloying elements. This kind of diagram has been extensively used for the design of the last generation of low modulus/high strength alloys, such as the "Gum metals" series [19].

Fig. 1 displays a stability map located through the Bo-Md coordinate (2.80–2.82, 2.40–2.45), based on the semi-empirical "d-electron" alloy design theory. The figure is a rough diagram to predict the deformation mechanism. Regarding this figure, the main features for design are related to the respective positions of transition lines where the transition between several deformation mechanisms of the β phase is predicted. Besides slip/twinning and Martensite start (Ms = RT, room temperature), there is also a TWIP/TRIP line (blue dashed line) located about halfway between the boundaries of the domains of stress-induced martensitic transformation and mechanical twinning, which means the potential occurrence of combined TRIP and TWIP effects when the composition of design alloy was located in the TWIP/TRIP line. It is worth noting that the colored areas in the figure are only a rough approximation, some alloys [20] also exhibit TWIP effect although not locating in the corresponding area. However, it's great potential to occur for stress-induced martensitic transformation and/or mechanical twinning, when the Bo-Md coordinate of the alloy located in this colored areas. Thus, in order to further investigate the "d-electron" alloy design theory for TWIP/TRIP effects, alloying development of a ternary composition by correlating two alloying vectors, Ti-Mo and Ti-Zr, is proposed to shift the alloying position along the design route. The "d-electron" coordinate at the (2.817, 2.427) near the Ti-12Mo position gives a composition of Ti-12Mo-5Zr (wt. %). Being close to Ti-12Mo, the as-designed alloy displays the potential TRIP/TWIP combined performance. Both mechanical behaviour and deformation microstructural features of the Ti-12Mo-5Zr alloy were investigated in this work.

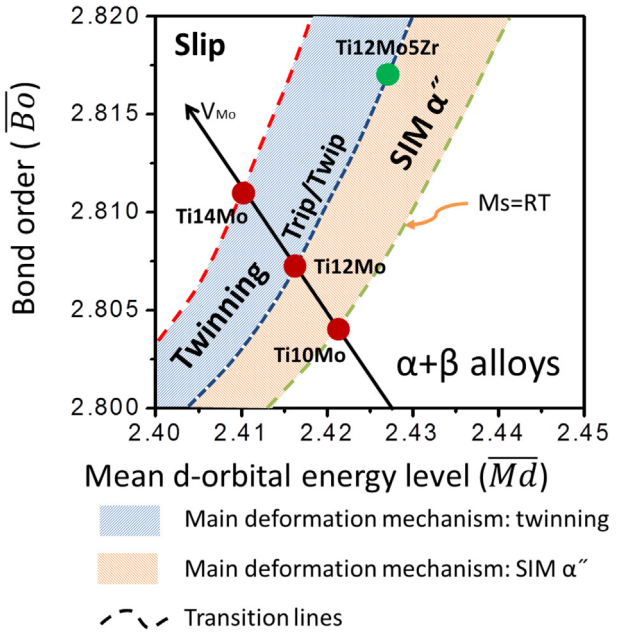

Fig. 1. The "d-electron" design map showing the position of the ternary Ti–12Mo–5Zr. A TRIP/TWIP line (blue dashed line) was located about halfway between the boundaries of the domains of stress-induced martensitic transformation and mechanical twinning, meaning the potential occurrence of combined TRIP and TWIP effects when the composition of design alloy was located in the TRIP/TWIP line. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

2.2. Experimental Procedures

The ternary Ti–12Mo-5Zr (wt%) alloy was fabricated by the arc-melting furnace under pure Ar atmosphere using pure titanium, molybdenum and zirconium. The alloy ingot about 3 kg was melted for five times, and flipped over each time before melting. Then, the ingot was homogenized at 1173 K for 72 ks under high vacuum of 10^{-4} Pa, followed by water quenching. The as-quenched ingot was heavily cold rolled to 0.5 mm in thickness at a reduction rate of > 95% at room temperature. From the as-rolled sheet, tensile specimens were mechanically prepared with gauge dimensions of 60 mm (length) × 5 mm (width) × 0.5 mm (thickness). The specimens were solution-treated (ST) at 1173 K for 1.8 ks under high vacuum atmosphere and subsequently water-quenched.

Tensile tests, including uniaxial loading and cyclic loading-unloading, were measured in tension on specimens at an initial strain rate of $10^{-3}\,s^{-1}$. An extensometer was used to precisely measure the deformation of the specimens. All tensile tests were performed along the rolling direction.

The phase constitutions of the specimens were characterized by X-ray diffraction (XRD) using Bruker D8 ADVANCE with CuKα radiation operating at 40 kV and 40 mA. Specimens deformed to different levels were then observed by optical microscopy and transmission electron microscopy (TEM). Specimens for OM were first mechanically polished on silicon carbide abrasive papers followed by a final polishing step with a colloidal silica suspension (particle size: 50 nm), and then chemically etched with a solution H_2O, HNO_3 and HF (5:3:1) (vol%). The TEM investigations were performed by using a JEOL 2100 microscope operating at 200 kV. Specimens for TEM observations were prepared by