

# **MICROSTRUCTURES AND MECHANICAL PROPERTIES OF THE TiAlNb ALLOYS**

Lan Huang

Department of Materials Science and Engineering, The University of Tennessee,  
Knoxville, TN 37996-2200

E-mail: [lh Huang2@utk.edu](mailto:lh Huang2@utk.edu); Telephone: (865) 974-0645; Fax: (865) 974-4115

P. K. Liaw

Department of Materials Science and Engineering, The University of Tennessee,  
Knoxville, TN 37996-2200

E-mail: [pliaw@utk.edu](mailto:pliaw@utk.edu); Telephone: (865) 974-6356;  
Fax: (865) 974-4115

and

C. T. Liu

Metals and Ceramics Division, Oak Ridge National Laboratory,  
Oak Ridge, TN 37831-6115

E-mail: [liuct@ornl.gov](mailto:liuct@ornl.gov); Telephone: (865) 574-4459; Fax: (865) 574-7659

## **ABSTRACT**

The TiAl alloys have been receiving considerable attentions because of their attractive properties, such as low densities, excellent high-temperature strengths, and good oxidation resistances. However, the TiAl alloys are quite brittle at room temperature and have relatively low fracture toughnesses. The relationship between the microstructures and mechanical properties of the intermetallic alloy has been investigated. With the addition of elements, such as niobium, tungsten, and boron, microstructures of the intermetallic alloys can be changed, and an enhancement in the mechanical properties of the alloy can be found. The addition of Nb is effective in improving the room-temperature ductilities, fracture toughnesses, elevated-temperature strength and oxidation resistances. The addition of W can result in an enhancement of mechanical properties, such as yield strengths, ultimate tensile strengths, and a refinement in microstructures. The boron addition in the lamellar TiAl alloys has a significant effect on room-temperature tensile ductilities.<sup>1-2</sup> The research plan and preliminary results of the Ti-Al-Nb-W-B alloys are discussed.

## **INTRODUCTION**

The TiAl-based alloys have attracted a great deal of interests for use in high-temperature structural applications due to their good elevated-temperature mechanical properties, low densities, and good creep and oxidation resistances. The initial application of these alloys was limited due to their poor fracture resistances at ambient temperatures. Efforts to enhance the ductility and refine the grain size in

these materials have focused on the microstructural control and alloying addition of B, Si, W, Cr, V, Mn, and Mo. In this program, a review on the microstructures and mechanical behaviors of the TiAl-based alloys has been conducted. The research plan and preliminary results of the TiAl-based alloys are presented.

## REVIEW

### Relationship between the microstructures and mechanical properties of TiAl-based alloys.

Three important microstructures of the TiAl-based alloys are: (1) fully lamellar (FL) microstructures,  $\alpha_2+\gamma$ ; (2) duplex microstructures (DP),  $\alpha_2+\gamma$  and  $\gamma$ ; and (3) near-gamma (NG) microstructures,  $\gamma$ . It is found that the  $\gamma$  phase is a very brittle phase, which leads the titanium-aluminide alloy to fracture. The TiAl-based alloys with a fully lamellar microstructure have the most balanced properties at both room and elevated temperatures.<sup>9</sup>

Fully lamellar structures are generally observed in cast conditions, and duplex structures are formed in thermomechanically-treated conditions. The FL microstructure consists of equiaxed polycrystalline grains with densely-packed lamellae. The lamellae are composed of  $\alpha_2$  plates interspersed between many  $\gamma$  plates. The DP microstructure, however, is made up of lamellar grains with single-phase  $\gamma$  grains distributed around them.<sup>10</sup>

The coarse FL structures with a grain size, ( $d$ ),  $d > 500 \mu\text{m}$ , exhibit adequate fracture toughnesses but usually poor tensile ductilities at room temperature. On the other hand, the DP structures with fine grain sizes ( $d < 50\mu\text{m}$ ) show adequate tensile ductilities but poor fracture toughnesses, and more importantly, poorer high-temperature strengths and creep resistances, as compared with the FL materials. The room-temperature tensile yield strength ( $\sigma_y$ ), fracture strength ( $\sigma_f$ ), and ductility ( $\delta$ ) of the TiAl-based alloys increase with decreasing the colony size of the fully-lamellar structure. Based on these correlations, a material with fine fully lamellar (FFL) microstructures would be expected to have balanced mechanical properties.<sup>11-14</sup>

Room-temperature (RT) tensile ductilities and toughnesses are two properties of considerable importance to the application of TiAl-based alloys. A great deal of research has been focused on optimizing the fully lamellar (FL) structure to have a fine grain size. This is because a FL structure with a fine grain size is known to have better balanced properties than the FL structure with a large grain size and the duplex (DP) one with a fine grain size.<sup>15-20</sup> Methods of refining fully lamellar structures includes:(1) solidification with grain refiner (e.g., borides)<sup>21,22</sup>; (2) rheocasting<sup>23,24</sup>; (3) supertransus processing (e.g. hot extrusion and forging of powders and ingots at a temperature,  $T$ , higher than the  $\alpha$  transus temperature,  $T_\alpha$ , or lower than  $T_\alpha$  but above the eutectoid temperature,  $T_e$  [ $\alpha \rightarrow \alpha_2+\gamma$ ]<sup>25-27</sup>; (4) thermomechanical treatment (e.g., forging plus heat treatment).<sup>28-30</sup> The third and fourth methods were widely used in previous studies, which involve mechanical treatments. The finest grain sizes reported

so far are those obtained the by hot extrusion of ingots and by hot forging plus heat treatments. Recently, an alternative method by which a coarse FL with a grain size of  $\sim 500 \mu\text{m}$  can be refined to  $\sim 10 \mu\text{m}$  merely by the rapid heat treatment.<sup>10</sup>

The fracture mechanisms in the duplex microstructures are the plasticity-induced grain-boundary decohesion and cleavage, while those in the lamellar microstructures are the interface delamination and cracking along the lamellae.<sup>31</sup> The lamellar microstructure is tougher than the equiaxed gamma or duplex microstructure because of the higher near-tip plasticity and an anisotropic composite-like fracture characteristic that yields a tortuous crack path, shear-ligament toughening, and an improved resistance-curve behavior. The tensile ductility of the lamellar microstructure increases with decreasing the colony size, while the fracture toughness shows a maximum at a large colony size.<sup>32</sup>

The initiation toughness,  $K_{IC}$ , of the lamellar TiAl-based alloys increases with increasing the grain size and the volume fraction of lamellar grains.<sup>32</sup> Both  $K_{IC}$  and the crack-growth toughness,  $K_S$ , increase with decreasing the lamellae spacing by affecting translamellar microcracking and the size of the shear ligaments.  $K_S$  increases with increasing the colony size, the volume fraction, and the width of crack-wake ligaments. At a large grain size,  $K_S$  depends on the grain size indirectly through the influence of the grain size on the ligament width. The tensile ductility in the TiAl-based alloys is limited by the instability of microcracks nucleated in the microstructure. The level of the tensile ductility depends on the  $K_{IC}$  value and the grain size. High fracture toughnesses can be attained in large-grained lamellar TiAl-based alloys with a fine lamellae spacing ( $< 2 \mu\text{m}$ ). The balanced properties of a moderate  $K_{IC}$  and plastic elongation ( $16 \text{ MPa}\sqrt{\text{m}}$  and 1.5%) can be attained in the fully-lamellar TiAl alloys with a size of approximately  $300 \mu\text{m}$  and a lamellae spacing of less than  $2 \mu\text{m}$ .<sup>33</sup>

### **Influence of Al, Nb, W, and B on microstructures and mechanical behavior of the TiAl-based alloys.**

The Al content in TiAl-based alloys has great effects on the microstructure and high-temperature strength.<sup>34</sup> With decreasing the Al content, the volume fraction of the  $\alpha_2$  phase increases. The average lamellae spacing decreases linearly with increasing the volume fraction of the  $\alpha_2$  phase. The best ductility typically occurs in the range of the 46-50 atomic percent (at.%) within the ductile Al range, and increasing Al generally decreases the fracture toughness. The lamellar colony size in the cast TiAl-based alloys (with 44–50 at.% Al and 1 at.% B) increases monotonically with increasing the Al concentration because the increased tendency to form the alpha phase with the increase of the Al content reduces the boron concentration in the liquid, thus reducing the role of boron in the grain refinement.<sup>35</sup>

The Nb content in the high Nb-containing TiAl-based alloys significantly increases the high-temperature strength. The Nb addition only shows slight effects on the volume fraction of the  $\alpha_2$  phase and the average lamellae spacing. The main effect of high Nb contents on high-temperature strengths relies on the increase of the value of  $\sigma_0$  in the Hall-Petch equation, as shown below:

$$\sigma_{0.2} = \sigma_0 + k_\lambda \lambda^{-1/2}$$

where  $\sigma_{0.2}$  is the 0.2% offset yield strength,  $\sigma_0$  and  $k_\lambda$  are material constants, and  $\lambda$  is the lamellae spacing. It means that the friction stress of moving dislocations arises mainly from the Peierls stress of the lattice, and the interactions between dislocations are much stronger than those for the TiAl-based alloys with less Nb contents.<sup>34</sup> The high Nb content also improves the high-temperature stability of microstructures of the TiAl-based alloys, resulting in the improvement of the high-temperature strength. The oxidation resistance of the TiAl-based alloys is improved with the Nb addition. The amount of Nb to be added is generally determined, depending on the oxidation resistance required. Nb slightly improves the creep resistance.

Tungsten was found to improve the creep properties significantly. The addition of W might act as a solid-solution strengthener so as to stabilize the  $\alpha_2+\gamma$  lamellar structure.<sup>36</sup> The motion of dislocations and/or interfaces could be impeded by  $\beta_2$  particles stabilized with tungsten. The addition of W also greatly improves the oxidation resistance.<sup>37</sup>

Alloying by boron in the TiAl-based alloys was proved to be an effective and economic method to achieve the grain refinement, reduce the lamellar colony size, and prevent the uncontrolled grain growth during heat treatments performed within the single-phase  $\alpha$ -field.<sup>38-40</sup> The effect of the boron addition on room-temperature tensile ductilities in the lamellar TiAl-based alloys depends predominately on the size of titanium-boride precipitates.<sup>40</sup> Alloys with fine titanium-boride precipitates have good ductilities, which is due to the refinement in the grain size induced by the boron addition in both wrought and cast conditions. Boron does not affect the yield strength while lowering the ductilities of the TiAl-based alloys containing  $> 0.10$  at. % B. Large titanium-boride precipitates proved to be detrimental to ductilities. Cracking along large titanium-boride precipitates can suppress the beneficial effect reflected from the grain refinement. Any refinement in titanium-boride precipitates, i.e., breaking down long titanium-boride precipitates by thermomechanical processing or limiting the boride-precipitate growth by fast cooling during solidification, will increase the ductilities significantly. The addition of  $> 0.5$  at.% of boron refines grain sizes, and improves strengths and workabilities.

## OBJECTIVE

The objectives of the research are to (1) design and fabricate the Ti-Al-Nb-W-B intermetallic alloys, (2) observe the phase composition of the intermetallic alloys after high-temperature heat treatments, (3) study and characterize the mechanical properties of the alloys, and (4) predict the relationship between the microstructures and mechanical behaviors. The present investigation will lead to a mechanistic understanding and theoretical modeling of processing and microstructural effects on the mechanical performance of these alloys, and a metallurgical way to improve their mechanical properties.

## RESEARCH PLANS

The research work will emphasize the processing and optimization of the microstructures of the Ti-Al-Nb-W-B intermetallic alloys for improving fatigue and fracture resistances. The materials used in this investigation have been prepared by drop-cast and powder-metallurgy techniques. Heat treatments will be conducted to refine the microstructures of the Ti-Al-Nb-W-B alloys. Fatigue and fracture properties will be developed as functions of processing methods and microstructures. To facilitate a mechanistic understanding of the fatigue-crack-initiation behavior, nondestructive-evaluation (NDE) techniques, such as replication methods, thermography, and scanning-electron microscopy (SEM), will be utilized to investigate crack-initiation mechanisms. Theoretical models will be attempted to predict fatigue-crack-initiation behavior. Moreover, the possibility for developing new extremely high-temperature intermetallic materials with good mechanical properties will be explored.

NDE techniques will be used to monitor the crack initiation and propagation process during the fracture-toughness and cyclic-fatigue experiments of the Ti-Al-Nb-W-B alloys. A series of fracture-toughness and fatigue specimens will be interrupted during testing at pre-determined points, followed by carefully cross-sectioning and studying by means of SEM. The fracture and fatigue-crack-propagation paths at various stages of testing will be statistically characterized, *e.g.*, the length along boundaries/interfaces, the cracking orientation with respect to loading directions, etc. It is expected that the fracture and fatigue-crack-propagation processes will be quantitatively investigated and modeled in the Ti-Al-Nb-W-B alloys.

The grain size, lamellae spacing, and colony size play a dominating role in controlling the fatigue and fracture characteristics of the Ti-Al-Nb-based alloys. Transmission-electron microscopy (TEM) will be utilized to characterize the fine structures of the grain boundaries and interfacial areas. It is planned to use a nanoindentation technique to probe mechanical properties in the grain-boundary areas.

On the basis of the above quantitative results, it will be attempted to conduct process modeling, which will relate processing parameters and alloy compositions to final microstructures. Furthermore, numerical simulations of the fracture processes in the Ti-Al-Nb-W-B systems will be performed to predict the fracture behavior and fatigue life under given loading, which will be used to optimize the microstructural design of the Ti-Al-Nb-W-B alloys with superior fatigue and fracture properties.

It is expected that the present investigation will lead to a mechanistic understanding and theoretical modeling of the processing, fatigue, and fracture behavior of Ti-Al-Nb-W-B systems, and a metallurgical way to improve their mechanical properties. The influence of processing parameters and microstructures on mechanical behavior of the Ti-Al-Nb-W-B systems will be emphasized.

## EXPERIMENTAL PROCEDURES

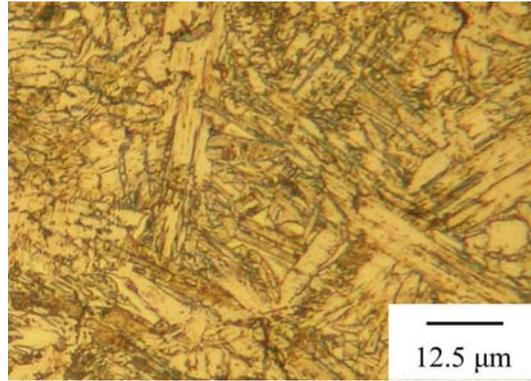
Niobium, tungsten, and boron are added to the arc-melted and drop-casted TiAl-based alloy, fabricated at Oak Ridge National Laboratory. The atomic percents of Nb, W, and B are 8.5%, 1.5%, and 0.05%, respectively. The Ti-44at.%Al-8.5at.%Nb-1.5at.%W-0.05at.%B sample was cut into four pieces, and capsulated into a quartz tube with argon inside. According to the Differential Scanning Calorimetry (DSC) graph, we are able to predict the phase-changing temperatures, and, thus, determine the proper heat-treatment temperatures. The four heat-treatment temperatures and related times are as follow: at 1,100<sup>0</sup>C for 48 hrs; at 1,240<sup>0</sup>C for 10 hrs; at 1,310<sup>0</sup>C for 5 hrs; and at 1,400<sup>0</sup>C for 2 hrs.

The newly fabricated TiAl-based alloys at Oak Ridge National Laboratory are: Ti-45Al-7Nb-0.15B; Ti-45Al-7Nb-0.15B-0.2W; Ti-45Al-7Nb-0.15B-0.4W; Ti-45Al-7Nb-0.15B-0.7W, in atomic percent. The atomic percents of the niobium, tungsten, and boron have been reduced. Since W and B are  $\beta$  phase stabilizers, the toughness of the newly fabricated materials should be improved. Heat treatments of the alloys have been scheduled. After capsulating all of the four pieces of alloys in one quartz tube, the samples are to be annealed at 1,100<sup>0</sup>C for 48 hrs, we will then section the 1,100<sup>0</sup>C-annealed alloys into five pieces for additional heat treatments at 900<sup>0</sup>C, 1,240<sup>0</sup>C, 1,310<sup>0</sup>C, and 1,400<sup>0</sup>C, respectively. At 900<sup>0</sup>C, alloy specimens will be annealed for 15 days, at 1,240<sup>0</sup>C for 10 hrs; 1,310<sup>0</sup>C for 5 hrs; and 1,400<sup>0</sup>C for 2 hrs.

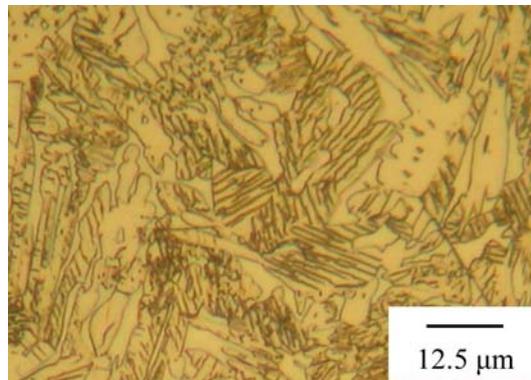
When heat-treatments of the alloys are finished, the microstructures of the alloys will be defined with the use of the optical microscopy, SEM, TEM, and an electron microprobe. Hardness tests on the heat-treated alloys will be performed. Since the strength of the material is controlled by the lamellae spacing, and the ductility is controlled by the grain size. The pertinent temperature and ways to produce the desired fully lamellae structures will be obtained. Mechanical experiments, such as tension, fatigue, and creep tests, will be performed, at both room and elevated temperatures.

## PRELIMINARY RESULTS

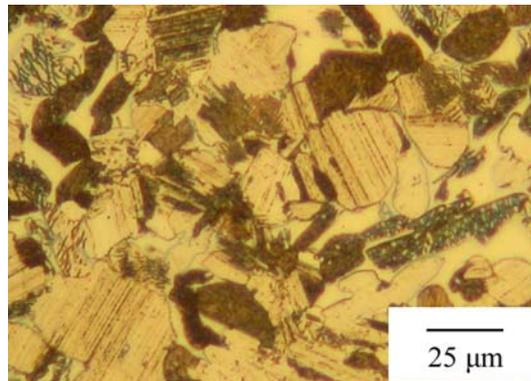
Microstructures of the Ti-44at.%Al-8.5at.%Nb-1.5at.%W-0.05at.%B sample, after the scheduled heat-treatments, are shown in Figs. 1-5, for the as-received, 1,100<sup>0</sup>C, 1,240<sup>0</sup>C, 1,310<sup>0</sup>C, and 1,400<sup>0</sup>C-annealed samples, respectively. This alloy contains mainly three phases,  $\alpha_2$ ,  $\delta$  and  $\beta$ , and the detailed analysis of the microstructures is in progress.



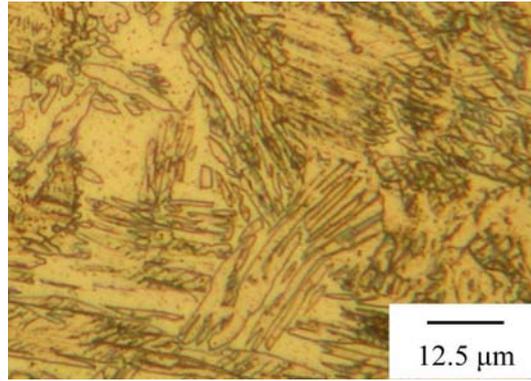
***Fig. 1 Microstructure of the As-received Ti-44at.%Al-8.5at.%Nb-1.5at.%W-0.05at.%B Alloy***  
The estimated phases are  $\alpha_2+\gamma$  and  $\gamma$ .



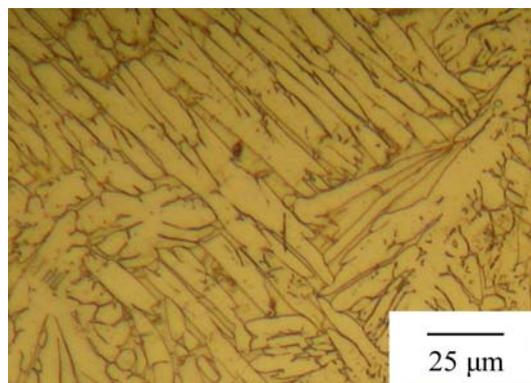
***Fig. 2 Microstructure of the Heat-treated Alloy, 1,100°C for 48 hrs***  
The estimated phases are  $\alpha_2+\gamma$  and  $\gamma$ .



***Fig. 3 Microstructure of the Heat-treated Alloy, 1,240°C for 10 hrs***  
The estimated phases are  $\alpha+\gamma$  and  $\gamma$ .



***Fig. 4 Microstructure of the Heat-treated Alloy, 1,310<sup>0</sup>C for 5 hrs***  
**The estimated phases are  $\alpha+\beta$  and  $\beta$ .**



***Fig. 5 Microstructure of the Heat-treated Alloy, 1,400<sup>0</sup>C for 2 hrs***  
**The estimated phase is  $\beta$ .**

## **SUMMARY**

The literature survey on the TiAl-based alloys has been completed. The heat treatments and microstructures of the Ti-44at.%Al-8.5at.%Nb-1.5at.%W-0.05at.%B alloy are being studied. Preliminary results on microstructure investigations have been reported. Research plans on the newly prepared TiAl-based alloys have been scheduled.

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