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Mechanical Properties and Crystal Structures of Hydrogenated Titanium Aluminides

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Structures of the Ti-Al-Zr alloys have been investigated by the X-ray diffractometer. Two ternary intermetallic compounds having the B2 and $L2_1$ structures were newly found in the present work. The B2 compound shows some compressive ductility, but the $L2_1$ compound shows no ductility at room temperature. Structural changes of the binary and ternary titanium aluminides exposed in a hydrogen atmosphere were investigated. No structural change was detected by hydrogenation of TiAl, but the transformation from the $D0_{19}$ to the fcc structure was observed in Ti_3Al. On the contrary, hydrogen induced amorphization was observed in the ternary aluminides with the B2 and $L2_1$ structures.

Keywords: Intermetallic compound, Titanium aluminide, Ductility, Hydrogenation.

INTRODUCTION

The titanium aluminides, Ti_3Al, TiAl and $TiAl_3$ are currently receiving considerable attention because of their potential as light weight, high temperature structural materials [1-6]. However, the use of these aluminides has been hindered by their lack of ductility at room temperature. Ternary alloying has overcome the problem of low temperature brittleness. For instance, the ductility of TiAl is improved by Mn, V and Nb additions [7-9]. On the other hand, one way of improving the room temperature ductility of Ti_3Al is adding the β-phase stabilizing elements such as Nb, Ta and V, resulting in alloys with aluminide + B2 structures, which have adequate low temperature ductility [10,11].

In the present work, the crystal structures of the Ti-Al-Zr alloys were examined in order to know whether the B2 compound is obtained in the Ti-Al alloys by alloying of Zr. The other problem in the use of the titanium aluminides in hydrogen containing environment is the possible hydrogen embrittlement. However, a little is known about the reaction products between the titanium aluminides and hydrogen gas. In the present work, the structures of the titanium aluminides after the exposure in a hydrogen atmosphere at elevated temperatures were examined in order to know the reaction between the titanium aluminide and hydrogen.

EXPERIMENTAL

The Ti-Zr-Al alloys, mainly along the $Ti_{50}Al_{50-x}Zr_x$ composition, were prepared by arc melting in an argon atmosphere. Structures of the arc-melted and hydrogenated samples were identified by the X-ray diffractometer using CuK_α radiation in combination with monochromator. The compression test of the ternary aluminides was done by the Instron testing machine at room temperature. Fracture surfaces were observed by scanning electron microscopy. Hydrogenation of the titanium aluminides was done by reacting the samples with 5 MPa H_2 for 86.4 ks at several temperatures.

RESULTS AND DISCUSSION

Formation of B2 and $L2_1$ compounds: The representative X-ray diffraction (XRD) patterns of the Ti-Al-Zr alloys are shown in Fig. 1. The XRD patterns of the $Ti_{50}Al_{50-x}Zr_x$ alloys indicate the five phases with the hcp, B2, $L2_1$, $D0_{19}$ and $L1_0$ structures. Among these, ternary compounds having the B2 and $L2_1$ structures are newly found in the present work. The formation ranges of the bcc type ternary aluminides in the arc melted state are shown in Fig. 2. The B2 phase is obtained around the $Ti_{45}Zr_{30}Al_{25}$ alloy as seen in this figure. The B2 compounds have so far been found in the Ti-Al alloys alloyed with the β-phase stabilizing elements such as V, Nb, Ta, *etc*. It is interesting to note that B2 compound is formed by alloying of Zr which has the complete solid solubility to Ti. The detailed alloying behavior of Zr in the TiAl compound has already been reported [12,13].

Fig. 3 shows a compressive stress strain curve of the Ti_2AlZr at room temperature. Ti_2ZrAl show 7 % compressive strain. A scanning electron micrograph of the fracture surface indicates that the transgranular fracture is dominant in Ti_2AlZr as shown in Fig. 4.

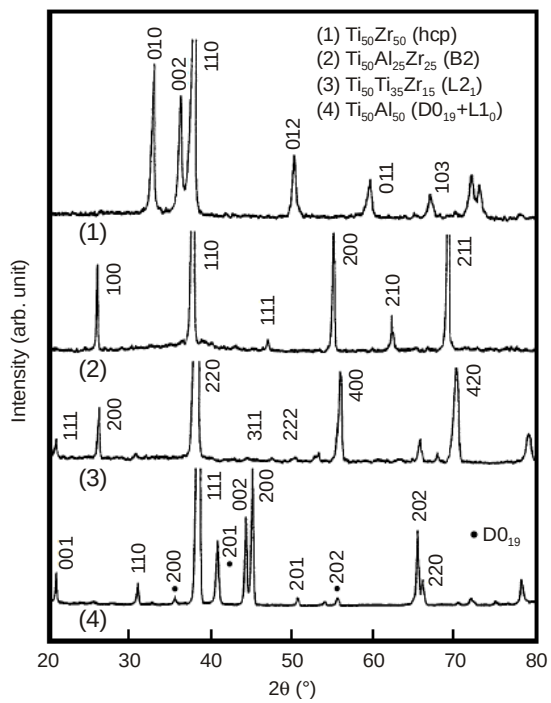

Fig. 1. X-ray diffraction patterns of $Ti_{50}Al_{50-x}Zr_x$ alloys

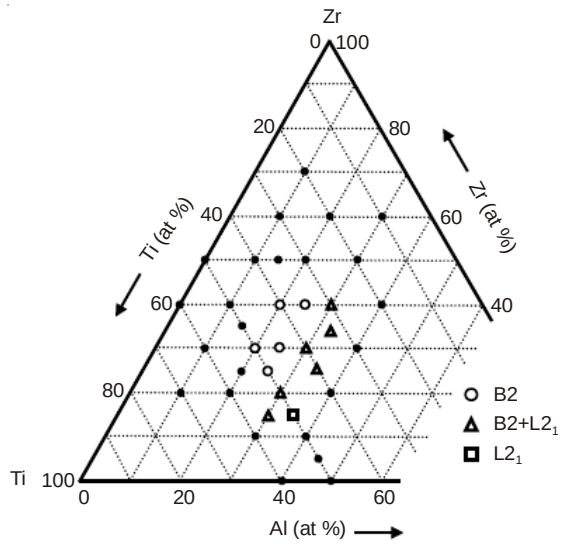

Fig. 2. Formation range of the B2 and $L2_1$ intermetallic compounds

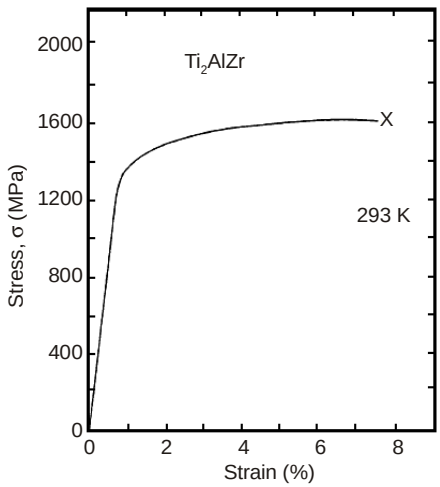

Fig. 3. A compressive stress strain curve of Ti_2AlZr

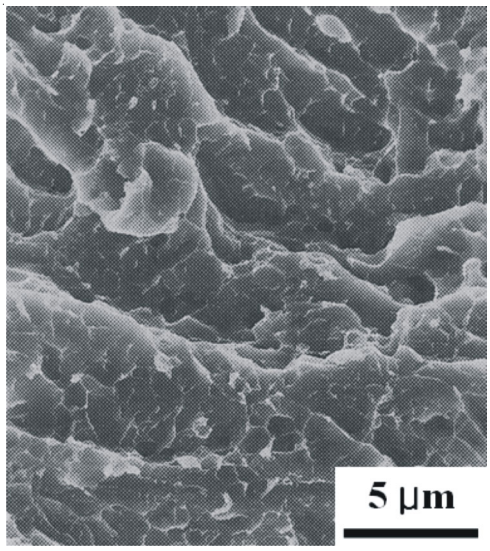

Fig. 4. Scanning electron micrograph of the fracture surface of Ti_2AlZr

On the contrary, $Ti_{50}Al_{35}Zr_{15}$ do not substantially show ductility. Much more investigations are necessary for understanding of the mechanical properties of the B2 compounds.

Structural changes of the binary and ternary aluminides by hydrogenation: The crystal structures of the intermetallic compounds, Ti_3Al, TiAl, Ti_2ZrAl and $Ti_{50}Al_{35}Zr_{15}$ after hydrogenation were examined using the X-ray diffractometer.

Figs. 5 and 6 show the XRD patterns of Ti_3Al and Ti_2AlZr hydrogenated at several temperatures, respectively. The XRD patterns indicate that Ti_3Al ($D0_{19}$) changes to fcc-$Ti_3AlH_{3.9}$ hydrogenation, although hydrogenation of Nd_3Ga, Sm_3Ga and R_3Al (R = a rare earth metal) with the $D0_{19}$ structures gives rise to hydrogen induced amorphization below about 400 K [14]. It is uncertain why hydrogen-induced amorphization does not occur in Ti_3Al. The XRD patterns of the hydrogenated at 300 K and 373 K show the broad halo characteristics of the amorphous phase.

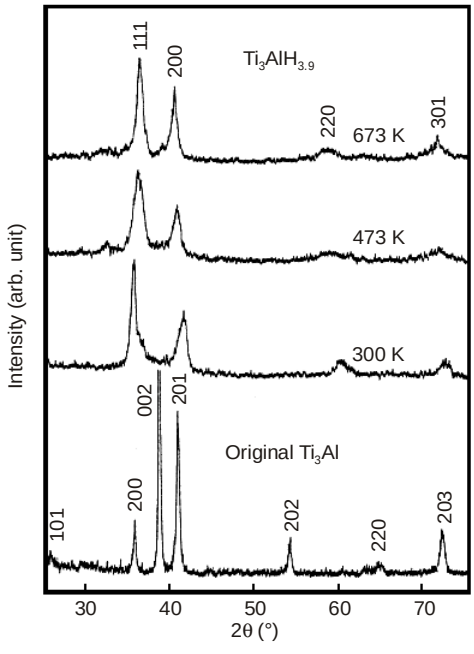

Fig. 5. X-ray diffraction patterns of Ti_3Al hydrogenated at several temperatures

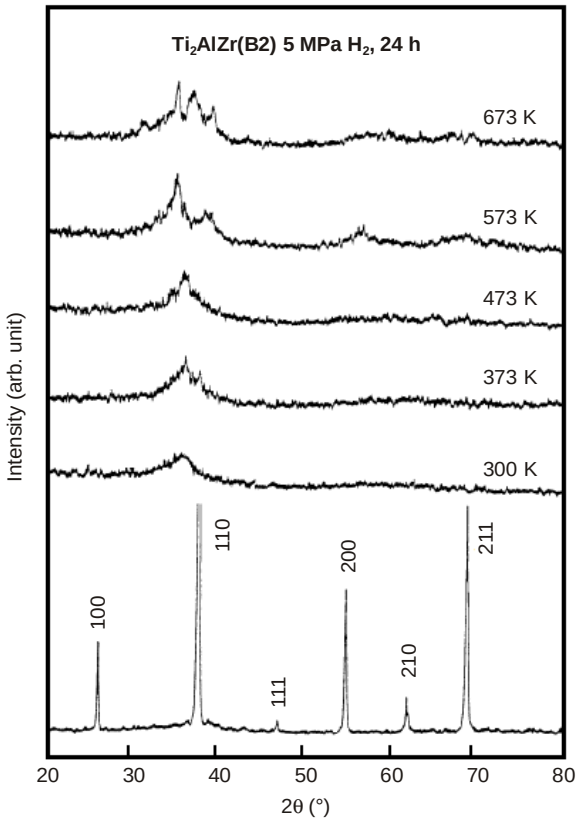

Fig. 6. X-ray diffraction patterns of Ti_2AlZr hydrogenated at several temperatures

Furthermore, the amorphous nature of these samples was confirmed by both transmission electron microscopy and differential scanning calorimetry. The XRD patterns of the samples hydrogenated above 400 K indicate the mixtures of the amorphous and the crystalline phases. Similarly, the $Ti_{50}Al_{35}Zr_{15}$ ($L2_1$) compound became amorphous by hydrogenation between 300 K and 500 K. Miyajima *et al*. [14] have reported that many intermetallic compounds having the C15, C23, $B8_2$, $D0_{19}$ and $L1_2$ structures amorphize by hydrogenation under appropriate conditions. According to our knowledge, hydrogen-induced amorphization in the bcc type intermetallic compounds is the first example. The elucidation of the mechanism of hydrogen induced amorphization in the B2 and $L2_1$ compounds is the subject for a future study. On the other hand, no structural change was detected by hydrogenation of TiAl, which indicates that there is no hydrogen embrittlement in TiAl.

Conclusion

Structures of the Ti-Al-Zr alloys have been investigated by the X-ray diffractometer. Two ternary intermetallic compounds having the B2 and $L2_1$ structures were newly found in the present work. The B2 compound shows some compressive ductility, but the $L2_1$ compound shows no ductility at room temperature. Structural changes of the binary and ternary titanium aluminides exposed in a hydrogen atmosphere were investigated. No structural change was detected by hydrogenation of TiAl, but the transformation from the $D0_{19}$ to the fcc structure was observed in Ti_3Al. On the contrary, hydrogen induced amorphization was observed in the ternary aluminides with the B2 and $L2_1$ structures.

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