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Structural analysis of C14-type Laves $TiMn_2$ alloy by XAFS

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Introduction

The hydrogen absorption property of $TiMn_2$ alloy depends on alloy composition severely in the same crystal structure. Repeat process of hydrogen absorption and desorption causes δ-TiH formation and several tens nanometer clustering in atom scale [1]. Hydrogen absorption capacity determined by PCT curves deteriorates with increasing the number of hydrogenation cycle, which is significant for Ti-60 at. % Mn. In this work, the change of interaction between constituent atoms in $TiMn_2$ alloy focusing on hydrogenation was investigated by EXAFS measurement.

Experimental

Four type samples of as-anneal, one cycle-hydrogenation, thirty cycles-hydrogenation and dehydrogenation at 673K after thirty cycles-hydrogenation were prepared for two alloys of Ti - 59 at. % Mn with superior hydrogenation property and Ti - 60 at. % Mn with inferior property. The samples other than as-anneal were supplied by pulverization in PCT experiments and the as-annealed samples were prepared by milling. The X-ray absorption measurement at 20K was carried out with synchrotron radiation using XAFS beam line BL-12C of KEK-PF.

Results

According to Fourier transforms |F(R)| of the EXAFS oscillation functions at the Mn K-edge, the intensity at 2.49Å monotonously decreases with the number of hydrogenation for Ti – 60 at. % Mn, while a drop of the intensity followed by a recovery of the same spectra intensity with increasing of hydrogenation cycles for Ti - 59 at. % Mn. Both samples show a full recovery of the intensity after dehydrogenation. The quantitative analysis of the spectra revealed that the Debye-Waller factors for the first nearest Mn-Mn and Mn-Ti correlation in Ti – 59 at. % Mn are almost constant independent of the process, while they increase with increasing of hydrogenation cycles in Ti – 60 at. % Mn as shown in Fig. 1. The result suggests that the distribution of the inter-atomic distance of Ti – 60 at. % Mn is relatively influenced by the hydrogenation compared with Ti – 59 at. % Mn. It is concluded that the hydrogen absorption capacity of $TiMn_2$ is closely related to the crystallinity of Laves phase.

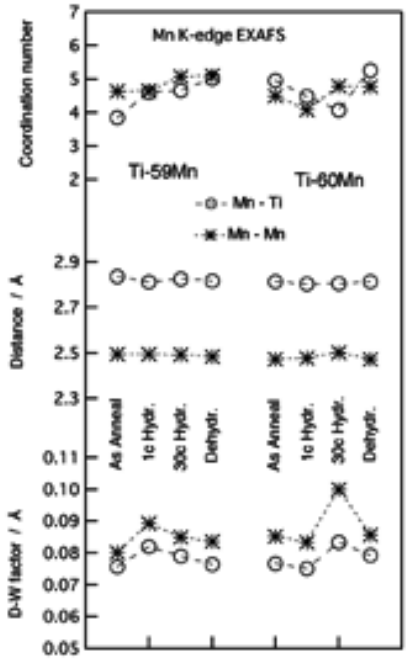

Fig. 1 The coordination number, distance and Debye-Waller factors of Mn-Mn and Mn-Ti in Ti –59 at. % Mn and Ti - 60 at. % Mn of as-anneal, one-cycle hydrogenation, thirty cycles-hydrogenation and dehydrogenation.

References

[1] S. Semboshi, N. Masahashi, S. Hanada: Acta Mater 49, 14 (2001) 927-935.

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