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利用課題名（日本語） :局所構造からのインタースティシャル元素の V-Ti-Mn 系 BCC 合金の耐久性に及ぼす影響の起源
Program Title (English) :The origin of the effects of interstitial elements on the cyclic stability of V–Ti–Mn bcc alloys from the local structure
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1. 概要（Summary ）

Metal hydrides can reversibly absorb and desorb a large amount of hydrogen at ambient conditions and this makes them attractive for energy storage application in fuel cell vehicles and large scale stationary energy storage systems. However, it often shows poor cyclic stability and it seems difficult to improve the cyclic stability of metal hydrides, especially solid solution alloys like V-based alloys with a body-centered cubic (bcc) structure. Our previous study suggested that a reduction in the reversible hydrogen storage capacity are due to the formation of a large number of lattice defects during hydrogen cycling and to have materials with excellent cyclic stability, we need to prevent the formation of lattice defects. Since it is known that dislocations can be pinned in some metals by nitrogen or carbon interstitial atoms, we decided to see how interstitial atoms affect on the cyclic stability of V-based bcc alloys.

2. 実験(目的,方法)（Experimental）

$V_{0.37}Ti_{0.33}Mn_{0.3}$ with and without a small amount of nitrogen (less than 2 at.%) were prepared. Our hydrogen cycling test result shows that the reversible hydrogen storage capacity of $V_{0.37}Ti_{0.33}Mn_{0.3}$ with nitrogen was reduced much more slowly than that of $V_{0.37}Ti_{0.33}Mn_{0.3}$ without nitrogen during hydrogen cycling. To find out the structural origin of the improved cyclic stability of nitrogen containing $V_{0.37}Ti_{0.33}Mn_{0.3}$, we prepared alloy, various monohydride and dihydride samples of the first cycle, monohydride samples (during the desorption process) of the 50th cycle and dihydride samples of the 101th cycle for both $V_{0.37}Ti_{0.33}Mn_{0.3}$ with and without nitrogen. Synchrotron X-ray total scattering experiment was carried out at BL22XU at SPring-8 using RA-PDF setup. The X-ray energy was 60.2017 keV.

3. 結果と考察(Results and Discussion)

Our diffraction data show that both samples undergo the same transitions during the hydrogenation process: they first show a solid solution phase with a bcc structure. Further increase in hydrogen gas pressure leads them to a monohydride phase with a tetragonal structure. For both cases, fully hydrogenated samples have a face-centered cubic structure. These results are consistent with previous work. Although both samples show bcc structure after the desorption process at the first cycle, their diffraction patterns after 50 cycles were not explained by a bcc structure alone any more. Further analyses on diffraction patterns as well as the atomic pair distribution function are underway.

4. その他・特記事項（Others）

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