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Sakine Khajavi, Mohammad Rajabi, Jacques Huot

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# Crystal structure of as-cast and heat-treated $Ti_{0.5}Zr_{0.5}(Mn_{1-x}Fe_x)Cr_1$, x=0, 0.2, 0.4

Sakine Khajavi[a,b], Mohammad Rajabi[a] and Jacques Huot[b*]

[a] Faculty of Materials and Industrial Engineering, Babol Noshirvani University of Technology, P.O.Box 47148-71167, Shariati Street, Babol, Iran

[b] Hydrogen Research Institute, Université du Québec à Trois-Rivières, 3351 des Forges, Trois-Rivières, G9A 5H7, Canada

## Abstract

The crystal structure of $AB_2$ metal hydride alloys of composition $Ti_{0.5}Zr_{0.5}(Mn_{1-x}Fe_x)Cr_1$, x=0, 0.2, 0.4 in the as-cast state and after heat treatment has been investigated. Based on SEM and X-ray diffraction results, all alloys were found to be multiphase. The best fitting of Rietveld refinement shows that the two main phases of each alloy have the same hexagonal structure with closely related lattice parameters and chemical composition. There is also some evidence that the microstrain values determined by Rietveld refinements are in fact an expression of composition variation within the phase and not a pure microstrain.

**Keywords**: Metal hydrides, $AB_2$ alloys, C14 crystal structure, Microstrain, Heat treatment, Rietveld refinement

## 1. Introduction

Hydrogen is considered to be a replacement for fossil fuels as an energy vector. However, in order to be widely used, a safe and inexpensive way to store hydrogen is needed. Conventional storage means such as high pressure and liquid hydrogen are presently the main ways to store hydrogen but each of them has limitations (high pressure, low temperature) and may not be suitable for a broad range of

* Corresponding author. Tel.: +1 819 376 5011x3576; fax: +1 819 376 5164.
E-mail address: jacques.huot@uqtr.ca (J. Huot).