Poster Presentation

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Study of Ti-V-Cr metal hydrides by neutron powder diffraction

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Metal hydrides are interesting materials from a fundamental as well as practical point of view. In particular, Ti-based BCC solid solutions are considered as promising candidates for mobile applications because of their high volumetric capacities and room temperature operation. However, the slow kinetics of the first hydrogenation, the so-called activation step, is an important hurdle in the use of these alloys for practical applications. It has recently been shown that doping a Ti-V-Cr composition with Zr7Ni10 leads to a fast activation kinetic without heating treatment [1]. We studied the effect of this doping on two new Ti-V-Cr compositions: 52Ti-12V-36Cr and 42Ti-21V-37Cr. Two different doping methods were investigated: i) a single-melt synthesis where the raw materials (i.e. Ti, V, Cr, Zr and Ni) chunks were mixed and arc-melted; ii) co-melt synthesis where 52Ti-12V-36Cr and 7Zr-10Ni were arc-melted independently and thereafter re-melted together. Using only X-ray diffraction for structural identification does not provide information about hydrogen localization. Therefore, neutron diffraction is essential for complete determination of this class of hydrides. The peculiarity of the present alloys is that, for neutron diffraction, the scattering lengths of the elements almost cancel. Therefore, the neutron pattern of as-cast alloy shows very small Bragg peaks but the advantage is that the hydride is very easy to see and analyze. We performed in-situ neutron diffraction experiments during dehydrogenation of these materials to see the transition from the dihydride to monohydride. These measurements were complementary to X-ray and synchrotron radiation diffraction and enabled a better crystal structure determination of these alloys

[1] *Miraglia, S., et al., Hydrogen-induced structural transformation in TiV0.8Cr1.2 studied by in situ neutron diffraction. Journal of Alloys and Compounds, 2007. 442(1–2): p. 49-54*

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