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Investigation of Entropy-Enthalpy Compensation Effect on the Ti-V-Cr system

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Hydrogen has attracted a permanent interest as a future energy carrier because of its high ignition power and pollution free nature. One problem facing the widespread of hydrogen as an energy carrier is storage. Presently the main ways to store hydrogen are in liquid form or as a high pressure gas. Both techniques have their drawbacks and new ways to store hydrogen at room temperature and low pressure should be found. One possible candidate is to store hydrogen in metal hydrides where hydrogen is chemically bonded to the metal atoms. Among various materials body centered cubic (BCC) solid solutions and alloys are found very promising due to their high volumetric storage capacity and relatively high gravimetric capacity. We have recently found that in Ti-V-Cr BCC solid solutions the enthalpy of hydrogenation is linearly related to the entropy change. This is the so-called enthalpy-entropy compensation. The aim of the present work is to investigate the entropy-enthalpy compensation effect by varying the elemental concentration of the Ti-V-Cr system. For this purpose, sample with different elemental concentration doped with 4wt.% of Zr7Ni10 have been synthesized by arc melting. The XRD patterns of as-cast samples confirm their BCC crystal structure. Lattice parameter and crystallite size were calculated by Rietveld analysis and hydrogenation studies were carried-out using a home-made hydrogen titration system. We found that for compositions Ti60V3Cr37, Ti52V12Cr36, Ti48V15Cr37, Ti42V21Cr37, and Ti33V30Cr37 the entropies and enthalpies are linearly correlated. The slope (Compensation temperature) was calculated to be 617 K. Possible explanations of this phenomenon will be discussed.

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