Body Centered Cubic Magnesium Niobium Hydride with Facile Room Temperature Absorption and Four Weight Percent Reversible Capacity

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We have synthesized a new metastable metal hydride with promising hydrogen storage properties. Body centered cubic (bcc) magnesium niobium hydride $(Mg_{0.75}Nb_{0.25})H_2$ possesses 4.5 wt.% hydrogen gravimetric density, with 4 wt.% being reversible. Volumetric hydrogen absorption measurements yield an enthalpy of hydride formation of -53 kJ/mol H_2, which indicates a significant thermodynamic destabilization relative to the baseline -77 kJ/mol H_2 for rutile MgH_2. The hydrogenation cycling kinetics are remarkable: At room temperature and 1 bar hydrogen it takes 30 minutes to absorb a 1.5 μm thick film at sorption cycle 1, and 1 minute at cycle 5. Reversible desorption is achieved in about 60 minutes at 175 °C. Using ab initio calculations we have examined the thermodynamic stability of metallic alloys with hexagonal close packed (hcp) versus bcc crystal structure. Moreover we have analyzed the formation energies of the alloy hydrides that are bcc, rutile or fluorite.

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