

# Energetics of atomic hydrogen absorption in C15-Fe<sub>2</sub>Zr Laves phases with ternary additions: A DFT study

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**Abstract:** The pseudo-potential Density Functional Theory (DFT) method using the Generalized Gradient Approximation (GGA) was applied to investigate hydrogen absorption trends in the cubic C15-ZrFe<sub>2</sub> Laves phase in the presence of several ternary additions. The effect of the ternary addition on the stability of the Laves phase was investigated. The relative stability of atomic hydrogen at various interstitial sites was determined taking into account the type of ternary addition for different H contents in the hydrides. The results were analyzed and particular attention was given to the formation and binding energies of hydrogen. It was found that hydrogen prefers the 96g site in the clean C15-Fe<sub>2</sub>Zr, and its absorption leads to decrease the heat of formation of the formed hydrides with occurrence of phase separation around 6H/fu. This effect was enhanced by the presence of ternary additions. Moreover, alloys with Be, V, Cr, Mn, Y and Tc elements at the Fe sites were found to absorb hydrogen up to 6H/fu. More interestingly, the cohesion of hydrogen atoms was found to be very sensitive to the third element nature. The hydrides with V, Y, and more particularly Tc and Ru have exhibited interesting energetics which would be very attractive for practical applications.

**Keywords :** Laves Phases, Hydrogen absorption, Atomic defects, Relative stability, DFT