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Energetics of atomic hydrogen absorption in C15-Fe2Zr Laves phases with ternary additions: A DFT study

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Abstract: The pseudo-potential Density Functional Theory (DFT) method using the GeneralizedGradient Approximation (GGA) was applied to investigate hydrogen absorption trends inthe cubic C15-ZrFe2 Laves phase in the presence of several ternary additions. The effect ofthe ternary addition on the stability of the Laves phase was investigated. The relativestability of atomic hydrogen at various interstitial sites was determined taking into accountthe type of ternary addition for different H contents in the hydrides. The results wereanalyzed and particular attention was given to the formation and binding energies ofhydrogen. It was found that hydrogen prefers the 96g site in the clean C15-Fe2Zr, and itsabsorption leads to decrease the heat of formation of the formed hydrides with occurrenceof phase separation around 6H/fu. This effect was enhanced by the presence of ternaryadditions. Moreover, alloys with Be, V, Cr, Mn, Y and Tc elements at the Fe sites were foundto absorb hydrogen up to 6H/fu. More interestingly, the cohesion of hydrogen atoms wasfound to be very sensitive to the third element nature. The hydrides with V, Y, and moreparticularly Tc and Ru have exhibited interesting energetics which would be very attractivefor practical applications.

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