HYDROGEN ADSORPTION ON beta-TiAl (001) AND Ni/TiAl (001) SURFACES

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Abstract

In this paper, we present first principles calculations of the energetic, electronic and magnetic properties of the variant termination of TiAl (001) and Ni/TiAl (001) surfaces with and without hydrogen atoms. The calculations have been performed within the density functional theory using full-potential linearized augmented plane wave method. The generalized gradient approximation (GGA) is utilized as the exchange-correlation energy. The octahedral site is the stable absorption site of H atom in the beta-TiAl system. This absorption reduces the cohesive energy of beta-TiAl system due to increase in the lattice constant. The surface energy for both TiAl (001) terminations is calculated. The stable adsorption site of H atoms on the variant termination of TiAl (001) surface is performed. The adsorption energy of hydrogen on Ti is more energetic than that on Al. The adsorption of H atom on both terminations of H/Ni/TiAl (001) is more preferable at the bridge site. The adsorption energies are enhanced on Ni atom due to the contraction between d-Ni bands and TiAl substrate band.

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