Ab-initio study of hydrogen storage in FeTi intermetallic

F. Z. BENTAYEB and A. KHADRAOUI

Laboratoire de Magnétisme et de Spectroscopie des Solides (LM2S), Dépt Phys., Faculté des Sciences, univ. Badji Mokhtar, B.P. 12 (23000) Annaba, Algeria

Due to its potential application as alternative energy, hydrogen storage in solid state has been considered to be one of the most promising energy sources. Experimental and theoretical studies have been devoted to the development of materials with high hydrogen capacity near ambient conditions. FeTi intermetallic with B_2 structure is one of the most interesting compounds for hydrogen storage due to its rapid reaction kinetics and high hydrogen absorbing ability.

The hydrogen storage and diffusion in Fe-Ti system are investigated. Structural and electronic properties of FeTi intermetallic and their hydrides are determined by using the density functional theory (DFT). Generalized gradient approximation (GGA) with the Perdew-Burke-Ernzehof (PBE) parameterization, as implemented in SIESTA (Spanish Initiative for Electronic Simulation with Thousands of Atoms), are considered.

The calculated equilibrium structural parameters and thermodynamic properties of FeTi intermetallic and its hydrides are in the range of available experimental and theoretical data. Absorption of hydrogen atoms within the FeTi lattice causes the increase in lattice constant and magnetic moment as well as a weakening in Fe-Ti bonds. The density of states (DOS), lattice data and bounding properties provide explanations for the role played by hydrogen in the chemical bond with the Ti and Fe constituents. From thermodynamic point of view, the intermetallic FeTi is good for hydrogen storage.

Keywords: Fe-Ti system; DFT calculation; Intermetallic hydrides; Hydrogen storage.