Etude ab initio des propriétés Structurales, Magnétique et Stabilité du système $Fe_2(Zr,Nb)$ dans les trois phases de Laves: C14 C15 et C36

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Abstract

The pseudopotential method (PP) Based on Density Functional Theory (DFT), using the Generalized Gradient Approximation (GGA) was applied to investigate the $Fe_2(Zr,Nb)$ system within the three Laves phases structures: Cubic C15, Hexagonal C14 and C36. The effects of Nb concentration on structural, magnetic and stability of the system were studied. The lattice parameters, bulk modulus and magnetic moments of the three phases were predicted and showed a significant dependence on Nb concentration. We evidenced the rigidity of the Fe_2Nb was higher than the Fe_2Zr one for C15, C14 and C36. The energetic phase diagram of the systems was also established by determining the heat formation and the stability of the alloys was discussed accordingly. The obtained results showed that the Laves phase have close formation energies which suggests that the C15, C14 and C36 phases can co-exist at low-temperature. In addition, the magnetic behavior was also established and the magnetic moments were found to be on Fe atoms. Consequently, these alloys were predicted to be ferromagnetic for all phases. The obtained results were in good agreement with available theoretical and experimental ones.

Keywords: Laves phases, Pseudopotential method, DFT, Heat of Formation, Stability.