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

L. Rabahi, A. Kellou, B. Alili

Abstract : The pseudopotential method (PP) Based on Density Functional Theory (DFT), using theGeneralized 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. Theeffects 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 werepredicted and showed a significant dependence on Nb concentration. We evidenced therigidity of the Fe2Nb was higher than the Fe2Zr one for C15, C14 and C36. The energeticphase diagram of the systems was also established by determining the heat formation and thestability of the alloys was discussed accordingly. The obtained results showed that the Lavesphase have close formation energies which suggests that the C15, C14 and C36 phases canco-exist at low-temperature. In addition, the magnetic behavior was also established and themagnetic moments were found to be on Fe atoms. Consequently, these alloys were predictedto be ferromagnetic for all phases. The obtained results were in good agreement with availabletheoretical and experimental ones.

Keywords : Laves Phases, Pseudopotential Method, DFT, Heat of Formation, Stability