Structural and thermal properties of $Fe_2(Zr,Nb)$ system in C15, C14 and C36 Laves phases:First-Principles study.

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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 ofNb concentration on structural, thermal and stability of the system were studied. The latticeparameters and bulk modulus of the three phases were predicted and showed a good agreement withthe available experimental data. 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 theheat formation of the different phases. The obtained results showed that the Laves phase have closeformation energies which suggests that the C15, C14 and C36 phases can co-exist at low-temperature. Finally, the temperature effect on the structural parameters, thermal expansions, heatcapacities and Debye temperatures are determined from the non-equilibrium Gibbs functions anddiscussed accordingly.

Keywords : Ab initio calculations, Pseudopotential Method, DFT, Laves Phases, Debye's Quasi-Harmonic Model