Theoretical study of structural and thermalproperties of Fe2 (Zr, Nb) Laves alloys

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Abstract : The aim of this is to use ab initio calculations(with the (PP) Pseudopotential method) to give newinsights on structural and thermal properties ofbinary and ternary C15-Laves Fe2(Zr,Nb) alloys. Thetemperature effects have been obtained using thequasi-harmonic Debye model exploiting the totalenergy calculations of the PP method. The main results show that:The structural properties obey to the Vegard's law,meaning that Fe_2(Zr, Nb) are quite ordered alloysindependent of the Zr/Nb ratio. In addition, The use of the quasi-harmonic Debye model wassuccessfully applied to determine the thermalproperties of the Fe_2(Zr, Nb) alloys in the 0-1000 Ktemperature range. The effect of temperature on bulkmodulii and volume expansions is important inFe2Nb while lesser in Fe_2Zr.

Keywords : Laves Phases, First-Principles calculations, DFT, Quasi-Harmonic Approximation, Debye's Model, Thermal Properties