

# Theoretical study of structural and thermal properties of Fe<sub>2</sub> (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 new insights on structural and thermal properties of binary and ternary C15-Laves Fe<sub>2</sub>(Zr,Nb) alloys. The temperature effects have been obtained using the quasi-harmonic Debye model exploiting the total energy calculations of the PP method. The main results show that: The structural properties obey to the Vegard's law, meaning that Fe<sub>2</sub>(Zr, Nb) are quite ordered alloys independent of the Zr/Nb ratio. In addition, The use of the quasi-harmonic Debye model was successfully applied to determine the thermal properties of the Fe<sub>2</sub>(Zr, Nb) alloys in the 0-1000 K temperature range. The effect of temperature on bulk modulus and volume expansions is important in Fe<sub>2</sub>Nb while lesser in Fe<sub>2</sub>Zr.

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