

# DFT calculations of structural magnetic and thermal properties of C15 C14 and C36 Laves phases in Fe-Nb-Zr

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**Abstract:** The Pseudo-Potential Density Functional Theory (PP-DFT) method is applied to investigate the C15, C14 and C36 Laves phases within the Fe-Nb-Zr system. The lattice parameters, bulk moduli, heats of formation and magnetic moments are predicted considering various spin configurations.  $ZrFe_2$  and  $Zr_{0.5}Nb_{0.5}Fe_2$  are found to be ferromagnetic in the C15 and C36 structures, respectively.  $NbFe_2$  is predicted to be ferrimagnetic in C36. The magnetic states dependency of these compounds on the volume compression shows interesting magnetic transition from the low to high spin state. This transition is more pronounced for  $NbFe_2$  and  $Zr_{0.5}Nb_{0.5}Fe_2$ . The thermal properties of  $NbFe_2$  and  $Zr_{0.5}Nb_{0.5}Fe_2$  are well predicted by using the quasi-harmonic Debye model. The obtained linear volume expansion for  $ZrFe_2$  is in excellent agreement with the experimental value at 800 K. The vibrational entropies of the studied alloys confirm the coexistence of the three Laves phases at high temperature.

**Keywords :** Laves Phases, Magnetism, Thermal Properties, DFT, Quasi-harmonic Debye model