

# Structure and stability of $\text{Fe}_2(\text{Zr}_{1-x}\text{Nb}_x)$ Laves Phases

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**Abstract :** The Laves phase structures (C15, C14 and C36) exist in a large number of binary and ternary intermetallic compounds of composition  $\text{AB}_2$ . Although they are well known since long time ago, there are still unsolved problems concerning the stability of the respective crystal structures. Therefore, it is difficult to predict which of the three structure types is the stable one for a given Laves phase compound. In this sense, several calculation methods have been successfully applied to predict the stable ground state structure of various Laves phases, but these calculations are restricted to the stoichiometric compositions and at 0 K. However in real systems the stability of Laves phase type is a function of temperature and composition and also different Laves phases types may coexist in a single system. This is the subject of the present work, where we applied the quasi harmonic approximation implemented on Gibbs2 program and the Ab initio pseudopotential method to study the temperature and composition-dependence transformations in the Laves phase  $\text{Fe}_2(\text{Zr}_{1-x}\text{Nb}_x)$  system. The results show a complex behavior with a cyclic variation of the stable structure types as function of temperature and Niobium concentration.

**Keywords :** Laves Phases, First-Principles calculations, Stability, Heat of Formation, Thermal Properties and Gibbs2 Program