Structure and stability of $Fe_2(Zr_{1-x}Nb_x)$ Laves Phases

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Abstract : The Laves phase structures (C15, C14 and C36) exist in a large number of binary andternary intermetallic compounds of composition AB_2. Although they are well known sincelong time ago, there are still unsolved problems concerning the stability of the respectivecrystal structures. Therefore, it is difficult to predict which of the three structure types is thestable one for a given laves phase compound. In this sense, several calculation methods havebeen 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 inreal systems the stability of laves phase type is a function of temperature and composition andalso different Laves phases types may coexist in a single system. This is the subject of thepresent work, where we applied the quasi harmonic approximation implemented on Gibbs2program and the Ab initio pseudopotential method to study the temperature and composition-dependence transformations in the Laves phase $Fe_2(Zr_{1-x},Nb_x)$ system. The results show acomplex behavior with a cyclic variation of the stable structure types as function oftemperature and Niobium concentration.

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