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

L. Rabahi, B. Alili, D. Bradai, T. Grosdidier, A. Kellou

Abstract: The Pseudo-Potential Density Functional Theory (PP-DFT) method is applied to investigate the C15, C14and C36 Laves phases within the Fe-Nb-Zr system. The lattice parameters, bulk moduli, heats of formationand magnetic moments are predicted considering various spin configurations. ZrFe2 andZr0.5Nb0.5Fe2 are found to be ferromagnetic in the C15 and C36 structures, respectively. NbFe2 is predictedto be ferrimagnetic in C36. The magnetic states dependency of these compounds on the volumecompression shows interesting magnetic transition from the low to high spin state. This transition ismore pronounced for NbFe2 and Zr0.5Nb0.5Fe2. The thermal properties of NbFe2 and Zr0.5Nb0.5Fe2 are wellpredicted by using the quasi-harmonic Debye model. The obtained linear volume expansion for ZrFe2 isin excellent agreement with the experimental value at 800 K. The vibrational entropies of the studiedalloys confirm the coexistence of the three Laves phases at high temperature.

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