

The Structural, Elastic, Thermal, Electronic, and Magnetic Properties of Intermetallic RMn_2Ge_2 (R=CA, Y, ND)

Authors : I. Benkaddour, Y. Benkaddour, A. Benk Addour

Abstract : The structural, elastic, Thermal, electronic, and magnetic properties of intermetallic RMn_2Ge_2 (R= Ca, Y, Nd) are investigated by density functional theory (DFT), using the full potential -linearised augmented plane wave method (FP-LAPW). In this approach, the local-density approximation (LDA) is used for the exchange-correlation (XC) potential. The equilibrium lattice constant and magnetic moment agree well with the experiment. The density of states shows that these phases are conductors, with contribution predominantly from the R and Mn d states. We have determined the elastic constants C_{11} , C_{12} , C_{13} , C_{44} , C_{33} , and C_{66} at ambient conditions in, which have not been established neither experimentally nor theoretically. Thermal properties, including the relative expansion coefficients and the heat capacity, have been estimated using a quasi-harmonic Debye model.

Keywords : RMn_2Ge_2 , intermetallic, first-principles, density of states, mechanical properties

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