Theoretical investigation of Structural, electronic, magnetic, thermodynamic and elastic properties of Heusler alloys Mn_2Al Z (Z= Cr,V).

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Abstract

In the recent years, the Heusler alloys are attracted the attention of many researchers because these materials are used in the spintronics applications. However we have investigated the structural, electronic, magnetic, thermodynamic and elastic properties of Mn_2Al Z (with Z= Cr,V). We employed in our calculation the full potential–linearized augmented plane wave (FP-LAPW) method within density functional theory (DFT) incorporated on wien2k code. Both approximations generalized gradient approximation (GGA) and local density approximation (LSDA) used to treat the exchange-correlation potential. In structural properties, we have defined the equilibrium lattice constants and bulk modulus by minimizing the total energy as function of unit cell volume. We applied Engel and Vosko approximation (EV-GGA) and modified Becke Johnson approximation (mBJ) to calculate the electronic band-structure, total and partial density of states and the electronic charge density. Also, we calculated the total and local magnetic moments of these alloys. We expand our study toward the thermal properties, so the dependence of the isothermal bulk modulus (B) and the adiabatic bulk modulus (Bs) on pressure and temperature are investigated with the quasi-harmonic Debye model. Also, the change of heat capacities at volume and pressure constants (C_v and C_p), the entropy, Debye temperature alpha and Gamma parameters have been studying as function as pressure and temperature. Finally, we calculated the elastic properties such as: the elastic constants, Young's modulus E, the anisotropy factor A, the adiabatic modulus of compressibility B_s and the shear modulus G (deformation resistance). The mechanical stability of Mn_2Al Z (Z= Cr,V) alloys are studied as function of the elastic constants.

Keywords: DFT; FP-LAPW; GGA; SLDA; EV-GGA; MBJ.