Ab initio study on the magnetic stability of Ni_2MnGe

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The electronic structure, ground state magnetic properties and thermal expansion of Ni_2MnGe Heusler alloy with cubic $L2_1$-type structure have been recently studied by first-principles methods. It was theoretically found that the magnetization of Ni_2MnGe shown a linear decreases with a hydrostatic pressure.

The main aim of a present study on the above-mentioned Heusler alloy is to investigate the influence of magnetic field on electronic structure and magnetic properties of the Ni_2MnGe. In a framework of DFT (density functional theory) methods it is possible to constrain the fixed value of the total magnetic moment (M) per unit cell. This fixed-spin-moment (FSM) method has been used in the full-potential nonorthogonal local orbital minimum basis (FPLO) scheme [www.fplo.de]. Thus, a particular ferromagnetic solution was forced on Ni_2MnGe. The obtained self-consistent total energy of the alloy is a function of two variables: the volume V and the total magnetic moment M. Only the minima with respect to M are called magnetic phase, since they do not require a magnetic field to maintain them and potentially could be stabilized by an applied stress such as an epitaxial stress. The obtained results of FSM study predicts that Ni_2MnGe in $L2_1$-structure has only one magnetic solution with the total magnetic moment of about 3.7 μ_B. Thus, the studied alloy has no metastable states.

9.7 cm

13.4 cm

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