Ab initio study on the magnetic stability of Ni$_2$MnGe
M. Pugaczowa-Michalska$^a$

$^a$Institute of Molecular Physics Polish Academy of Science, Smoluchowskiego 17, 60-179 Poznań, Poland

The electronic structure, ground state magnetic properties and thermal expansion of Ni$_2$MnGe 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$_2$MnGe 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$_2$MnGe. 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$_2$MnGe. 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$_2$MnGe 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.

Subject category :
3. Magnetic Structure and Dynamics

Presentation mode :
poster

Corresponding author :
Maria Pugaczowa-Michalska

Address for correspondence :
IFM PAN
ul.Smoluchowskiego 17
60-179 Poznań

Email address :
maria@ifmpan.poznan.pl