AB INITIO INVESTIGATION OF STRUCTURE AND MAGNETIC PROPERTIES OF Ni_2MnGa AND Co_2MnGa COMPOUNDS

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Half-metallic ferromagnets have been produced and studied as ideal candidates for the magnetoelectronic and spintronic devices. Among many half-metallic ferromagnets special attention has been drown on Heusler alloys such as Ni_2MnGa and Co_2MnGa that show high Curie temperature and high spin polarization [1]. Several studies by means of X-ray and neutron diffraction measurements indicate that the alloys present $L2_1$ structures with mainly ferromagnetic ordering [2]. However, R. J. Kim and et al. found a well-ordered crystalline state, a disordered state and crystalline state with an intermediate order and exhibited influence of the structural order on the physical properties of the Co_2MnGa films [3]. The similar phenomena for Ni_2MnGa are described in work [4]. The results of our recent theoretical investigations of these compounds consist of eight lattices prove the presence of the disordered and ordered structures in the above compounds. The results obtained indicate Co_2MnGa and Ni_2MnGa as compounds possessed a cubic lattice. However, the 8 cubic lattices form the ordered structure in Co_2MnGa and disordered in Ni_2MnGa. 'Disordered' means that the cubic lattices of the Ni compound are shifted in respect each other (Fig.1)

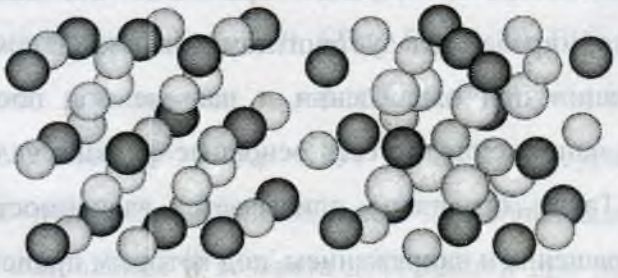

Figure1. View of the Co_2MnGa structure investigated on the left and that of Ni_2MnGa on the right. Co or Ni is marked by light grey cycle, Ga- grey Mn- black

The analysis of the charge distribution, bond orders and lengths indicates different electronic structure of the compounds although their magnetic properties are similar [5]. Hence the questions arisen: do the obtained structures take place in the periodic structure, i.e. the structures obtained is translated; do the disorder obtained in experiments is related with cubic cell shift as it is found in the case of Ni compounds; are the charge and spin distributions of the above structures took place in periodic structure, too; are differences of the magnetic properties of these compounds investigated obtained in the periodic structures.

To answer the above questions we perform investigation of the periodic structure of the Co_2MnGa and Ni_2MnGa compound by using state-of-the-art computational ab-initio methods.

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