INVESTIGATION OF ELECTRONIC STRUCTURE OF HEUSLER ALLOYS: CUBIC AND TETRAGONAL CELLS

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Abstract – The work is devoted to the Heusler alloys as a candidate for applications in spintronics. On the basis of experimental studies the electronic structure of these alloys by computer simulations were carried out. Hence, the purpose of our work is to simulate and to explain the variety of structural properties of the Ni_2MnGa and Co_2MnGa compounds by using state-of-the-art computational ab-initio methods. The total energy calculations for the cubic and the tetragonal structures, band structure and its nature and magnetizability have the compounds are investigated. The obtained results will explain the dependence of the magnetic properties of the alloys on the geometrical structure as well influence of Co and Ni on these properties.

I. INTRODUCTION

Half-metallic ferromagnetic alloy have been studied as a candidates for the metal-based the spintronic-logic devices. Among many half-metallic ferromagnetic materials special attention has been done on Heusler alloys such as Ni_2MnGa and Co_2MnGa that show high Curie temperature and high spin polarization [1-5]. Several studies by means of X-ray and neutron diffraction measurements indicate that the alloys present $L2_1$ structures with mainly ferromagnetic ordering [6]. 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 structural order on the physical properties of the Co_2MnGa films [7]. The similar phenomena for the Ni_2MnGa are described in work [8]. More often, the substrate temperature is mentioned as having dramatic effects on the structural ordering and magnetic properties, however the effects of structural disorder on the various physical properties of these alloys are not fully understood. Moreover, the dependence of electronic structure on the alloy geometrical structure is insufficiently described although it could be the main reason to understand what can be responsible for many of the alloy properties.

Hence, the purpose of our work is to simulate and to explain the variety of structural properties of the Ni_2MnGa and Co_2MnGa compounds by using state-of-the-art computational ab-initio methods. The total energy calculations for the cubic and the tetragonal structures, band structure and its nature and magnetizability have the compounds are investigated. The obtained results will explain the dependence of the magnetic properties of the alloys on the geometrical structure as well influence of Co and Ni on these properties.

II. RESULTS

At present time quantum mechanical investigation of the Ni_2MnGa and Co_2MnGa possessing $L2_1$ structure were investigated. The views of the structures are presented in Fig. 1. The aim of the first investigation is to establish how the electronic properties of the alloys are changed when the Ni atoms in the lattice are changed by the Co atoms and vice versa.

Let us to remember that the Co and Ni atoms are different not only due to different electrons but also due to electronic configuration. The Co atom electronic configuration is $[Ar]4s^23d^7$ while Ni one is $[Ar]4s^23d^8$ and $[Ar]4s^13d^9$. Thus, there is some disagreement as to which the Ni electronic configuration should be considered the lowest energy configuration [9-11]. Of course, the isolated atoms and atoms in the compounds electronic configurations are different, but it could be essential to explain properties of the compound that is related with charge redistribution.

First, our investigated systems are open shell systems due to odd number of the Mn atoms. However, the highest electronegativity numbers, what indicate ability an element attract electrons toward it, are the Co and Ni atoms in the investigated compounds. Indeed in our investigated Ni_2MnGa compound the largest negative charge possesses Ni atoms, while charge of the Ga and Mn atoms is positive or negative (Fig.1). Moreover, the charge is not distributed equally that leads to appearance of

the high dipole moment (144.67 Deby) with large dy component (dy=139.63 Debye) that could indicate concentration of the negative charge and, as consequence, large uncompensated spin presence.

Indeed, the largest spin densities are obtained on the Mn atoms that electronegativity is smaller than Ni (Fig. 2). Thus, we predict, that it could be happens due to an electronic configuration changes and different oxidation states of the atom presented in the different places of the investigated compound. Hence, the Ni atoms attract the electrons to form chemical bonds, while an additional electron is located on Mn atoms mostly due to their configuration of d orbital [12]. It is necessary to remember that only Mn atom could have oxidative state such as -1, -2 or -3, while other atoms of the compound oxidative state is positive and indicate that theses atoms may not accept an additional electron. It is necessary to pay attention to different spin densities on the Mn atoms located in different places of the investigated compound (Fig.2). Thus, the results obtained indicate geometrical structure of the compound is important for their magnetic properties.

The above conclusion is confirmed by the investigation results of the $Ni_2Mn_{0.375}Ga_{0.625}$ compound (Fig.3). It is clear to see the largest spin density on the Ni atom, when Mn atom is changed by Ga.

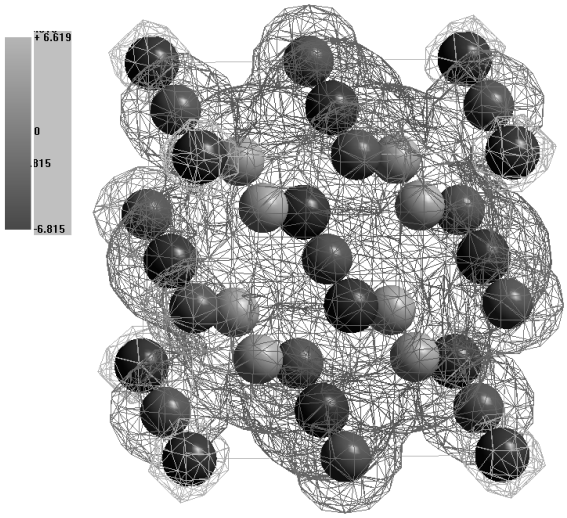

Figure 1. The 3D Mapped Isosurface of Electrostatic Potential of the Ni_2MnGa compound. The light grey colored bubble is Ni, dark grey – Mn and black –Ga

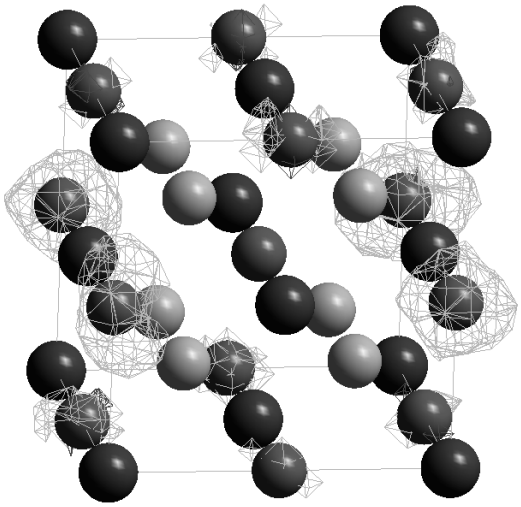

Figure 2. The 3D Isosurface of Total Spin Density. The light grey colored bubble is Ni, dark grey – Mn and black –Ga.

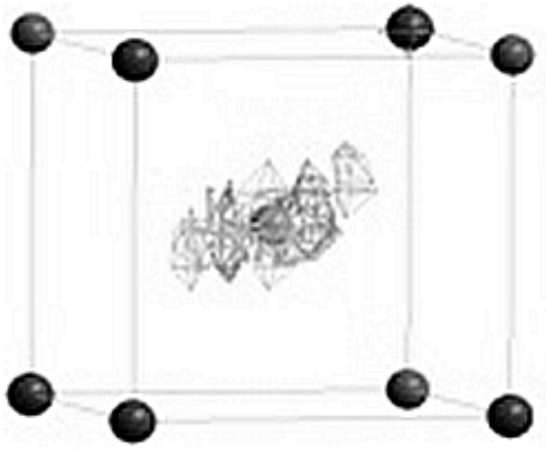

Figure 3. The 3D Isosurface of f the total spin $Ni_2Mn_{0.375}Ga_{0.625}$ alloy. The light grey colored bubble is Ni, dark grey – Mn and black –Ga.

It is necessary to mention that the last one system is closed shell system, i.e. there is no free electron. In this case, the Ni atom possessing the highest electronegativity numbers attracts electrons toward it. However the spin density on the Ni atom is equal to 0 approximately due to several reasons: the attracted electrons may form chemical bonds and there is no the free electron

CONCLUSION

The primary results of the investigations exhibited that the spin density of the Ni_2MnGa alloy are atom placement depended.

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