acta physica slovaca vol. 46 No. 2, 133 – 135 April 1996

MAGNETISM IN Rh_2MnX (X = Al, Ga, In) HEUSLER ALLOYS[1]

M. Pugacheva, A.Szajek[2], A. Jezierski
Institute of Molecular Physics, Polish Academy of Sciences, ul.Smoluchowskiego 17, 60-179 Poznan, Poland

Received 31 July 1995, accepted 8 February 1996

The electronic structure and magnetic properties of ordered Rh_2MnX (X = Al, Ga, In) Heusler type alloys have been studied by the LMTO method. The calculated total magnetic moments are close to the experimental values and the main contribution give Mn atoms.

1. Introduction

In this paper we are interested in the magnetic properties of the Rh_2MnX Heusler alloys (where X is one of the elements from III B group). In the last years the magnetic properties of Heusler alloys had been extensively examined both theoretically [1-3] and experimentally [4].

Heusler alloys are considered as ternary intermetallic compounds usually containing Mn atom and as systems of localised magnetic moments [1]. For X from the group III B the compounds predominantly are ferromagnetic with low Curie temperatures and low magnetic moments at low temperatures. The experimental data of the magnetic moments [3] show that the Rh_2MnX (with X = Al, Ga, In) alloys are ferromagnetically ordered.

The present systems have the B2 type structure with the double lattice constant. The rhodium atoms occupy the corner sites of the simple cubic sublattice and other atoms (Mn and X) occupy the second sublattice, i.e. they are located in the body centre position of the rhodium sublattice.

In our theoretical investigation of the mentioned Heusler alloys we calculate the electronic structures and magnetic moments.

[1] Presented at 9th Czech and Slovak conference on magnetism, Košice, Slovakia, August 28-30 1995
[2] emailszajek@ifmpan.poznan.pl

0323-0465/96

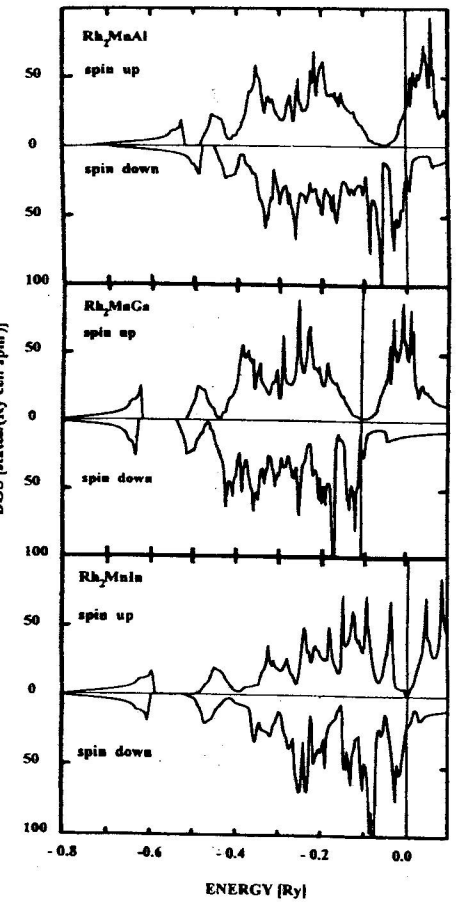

Fig.1. The spin-polarised DOS for Rh_2MnX (X = Al, Ga, In).

2. Method

The electronic structures were calculated using the self-consistent spin-polarised TB LMTO [5] method in the atomic-sphere-approximation (ASA) with exchange correlation potential in the form proposed by von Barth and Hedin [6]. We assume, that the initial electronic configurations for the atoms are: Rh - core $4d^85s^1$, Mn - core + $3d^54s^2$, Al - core + $2s^2p^1$, Ga - core + $3s^2p^1$, In -core + $4s^2p^1$ and we take the experimental values of the lattice parameters, namely a = 11.352, 11.444 and 11.885 a.u. for X =Al, Ga, In, respectively. Our further assumption concerns with the values of the Wigner-Seitz (W-S) radii for Rh, Mn and X atoms. In the spirit of the ASA the W-S cell is replaced by a sphere with the same volume. We take however the different values of the W-S radii for Rh, Mn and X atoms. The following relation is used $\sum_n (S_n / S_{av})^3 =$, where summation is over all type of atoms in the cell and Sav is the average W-S

radius. The average W-S radius is determined by $S_{av} = a (3/4\pi N)^{1/3}$, where N is the number of atoms in the cell and a denotes the experimental lattice constant.

3. Results and Discussion

Our calculations have shown that the Rh_2MnX alloys are ferromagnetically ordered. The energies of the ferromagnetic states are lower that the energy of paramagnetic one for all of three systems. This is in agreement with experiment [3]. The calculated densities of electronic states (DOS) of the Rh_2MnX ordered alloys for the both spin directions are shown in fig.1. To understand the role of Mn atoms we compare our DOS calculated for Rh_2MnX with those of obtained for isostructural RhX compounds using the ASW method [7]. Due to Mn alloying the separation of s-states from p-d - states which originates from hybridisation of the d- states of the Mn atom and p-states of the X atoms is observed. This separation is responsible for the appearance of a gap. The occurrence of the gap depends on the distance between the atoms and the type of ordering [8,9]. The total magnetic moments of the examined Heusler alloys are m =4.04, 4.10, 4.11 (μ_B/f.u. for X = Al, Ga, In, respectively. The main contribution to the total magnetic moment give the Mn atoms (m = 3.38, 3.42 and 3.45 μ_B). The values of the local magnetic moment on the Rh atoms are about 0.35 μ_B. The contributions to the total magnetic moment from X atoms are negligible, but the type of X atom has an indirect influence on the magnetic moment of the Mn atom due to the change of the local environment and thus the electronic structure.

References

[1] A.R. Williams, V.L.Moruzzi, C.D. Gelatt, Kuebler: *J. Magn. Magn. Mat.* **31-34** (1983) 88

[2] S. Ishida, Y. Kubo, J. Ishida, S. Asano: *J. Phys. Soc. Jpn.* **48** (1980) 814

[3] J. Kuebler, A.R. Williams, C.B. Sommers: *Phys. Rev.* **B28** (1983) 1745

[4] J.C. Suits: *Phys. Rev.* **B14** (1976) 4131

[5] O.K. Andersen, O. Jepsen, M.Sob: in: *Electronic Structure and Its Applications* Ed. M.S. Yussouff (Springer, Berlin, 1987) p.2.

[6] U. von Barth, L. Hedin: *J. Phys.* **C 5** (1972) 1629

[7] B.H. Verbeek, H.W.A. Rompa, P.K. Larsen, M.S. Methfessel, F.M.Mueller: *Phys. Rev.* **B28** (1983) 6774

[8] S. Ishida, S. Asano, J. Ishida: *J. Phys. Soc. Jpn.* **53** (1984) 2718

[9] A. Jezierski, G. Borstel: *Physica* **B205** (1995) 397