Magnetic and electronic properties of the compound $Y(Co,Fe)_5$ calculated by the augmented spherical wave method

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Energy band structure and density of states of the compound $Y(Co,Fe)_5$ were obtained by the augmented spherical wave method. Also the localization of the magnetic moment inside the unit cell, the effect of pressure and the substitution of Co atoms by Fe atoms were studied at the temperature of 0 K. Metallic Co showed a magnetic moment of 1.5 μ_B while metallic Y showed its nonmagnetic behavior. Inside the compound YCo_5 the Y atom had a contribution of –0.3 μ_B to the total magnetization of the unit cell. A negative pressure caused the change of the Fermi energy and the modification of the magnetic moment. With a big enough positive pressure the total magnetic moment dropped to zero. The substitution of Co by Fe caused a change in the compound from strong ferromagnetic to soft ferromagnetic.

Introduction

Rare earth-3d transition metal intermetallic compounds such as $Nd_2Fe_{14}B$ and $SmCo_5$, are the magnets of better performance nowadays. They combine strong anisotropy energy, caused mainly by the rare earth sublattice, with saturation magnetization reasonably high provided by the transition metal atoms. Among them, the compound YCo_5 stands out because of its high Curie temperature and high magnetocrystalline anisotropy and it has been studied theoretically [1-9] and experimentally [10-15] by several methods .

The YCo_5 intermetallic compound crystallizes in the hexagonal $CaCu_5$ structure, space group no. 191 (P6/mmm) with Y occupying 1a site and Co occupying two non-equivalent sites 2c and 3g (Fig. 1).

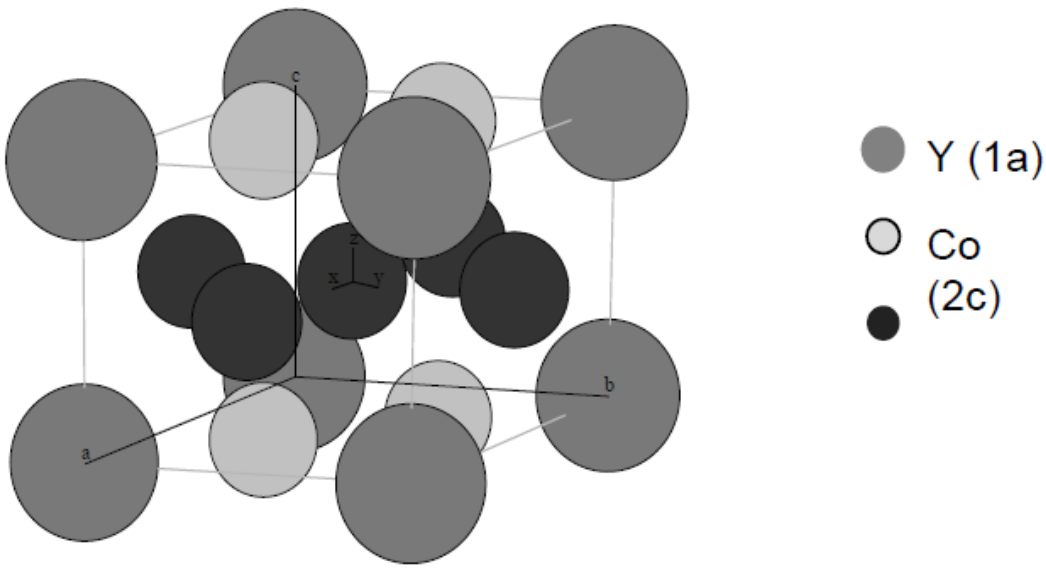

Fig. 1. The YCo_5 unit cell.

As the pure YFe_5 intermetallic compound cannot be experimentally sinthesized, pseudobinaries $Y(Co,Fe)_5$ have been synthesized and studied, finding out that all of them have hexagonal structure [1]. The relative Fe content which can be substituted for Co is up to 20% in YCo_5 [16]. Neutron diffraction studies revealed that the Fe atoms preferentially occupy the 3g site while the Co atoms prefer the 2c site in the $Y(Co,Fe)_5$ structure [17].

In this work we studied the energy band structure, density of states and localization of the magnetic moments inside the unit cell of the compound YCo_5 and the pseudobinaries YFe_2Co_3, YCo_2Fe_3 and YFe_5 obtained by the augmented spherical wave method in the framework of the local density approximation. The effect of positive and negative pressure on the YCo_5 structure was also studied at

the temperature of 0 K.

Method of calculation

Spin polarized calculations were carried out using density functional theory (DFT) in the local density approximation (LDA) developed by Hohenberg, Kohn and Sham [18, 19]. The ASW program developed by J. Kübler was used in the calculations [20]. This program use the ASW method, developed by Williams, et.al [21], to solve the one-particle Kohn-Sham equations. As many other augmentation methods, it's based on a special form of Slater's muffin-tin approximation (MTA) [22], named the atomic sphere approximation (ASA). Invented by Andersen [23,24], the ASA states that the MT spheres should be enlarged and even slighty overlapped to fill the space completely, so the sum of the atomic sphere volumes is equal to the cell volume. As spin-orbit coupling was not included in the calculations, the magnetocrystalline anisotropy energy was not calculated.

Experimental lattice parameters were used for the calculations shown in Table 1. There is not available experimental information on the lattice parameters of the pseudobinaries YCo_2Fe_3 and YFe_2Co_3, so those of the YCo_5 structure were used. In the irreducible Brillouin zones 576 k-points were used and convergence was achieved when the difference in charge was $\Delta Q<10^{-5}$ and the total variational energy change was $\Delta E<10^{-5}$ Ry.

Table 1. Experimental lattice parameters used for calculations.

	Space Group	Crystalline structure	Lattice parameters [a.u.]		
			A	c	c/a
Fe[25]	229 Im3m	bcc	2.8665	2.8665	1.0000
Co[26]	194 $P6_3/mmc$	hcp	2.5071	4.0686	1.6228
Y[27]	194 $P6_3/mmc$	hcp	3.6474	5.7306	1.5711
YCo_5[28]	191 P6/mmm	$CaCu_5$ (hex:ab_2b_3)	4.9480	3.9750	0.8033

The ASW program uses a δ parameter which is an empirical parameter that allows to scale the size of the atomic spheres. It is like pressure. When δ is zero, the program supplies an atomic volume that, upon iteration, will result in the lattice constant which approximately minimizes the total energy. On the other side, a small negative δ value, like a negative pressure, will result in a larger lattice constant, and a small positive δ value, like a positive pressure, will result in a smaller lattice constant [20].

Results and Discussion

First density of states (DOS) and band structure calculations were carried out for the pure elements Y, Co and Fe (see table 1 for crystallographic information). The total magnetic moment per atom calculated for the pure elements was 2.17 μ_B for Fe and 1.53 μ_B for Co. Y showed no magnetic moment. This results are nearly similar to those reported by Skomski and Coey [10] of 2.23 μ_B for Fe and 1.73 μ_B for Co. The energy values are given with respect to zero Fermi energy ($E_F = 0$).

Fig. 2 shows the calculated spin-up and spin-down partial and total density of states of the YCo_5 intermetallic compound. It can be observed that the spin-up band is completely filled but the spin-down is not, which is typical for strong ferromagnets.

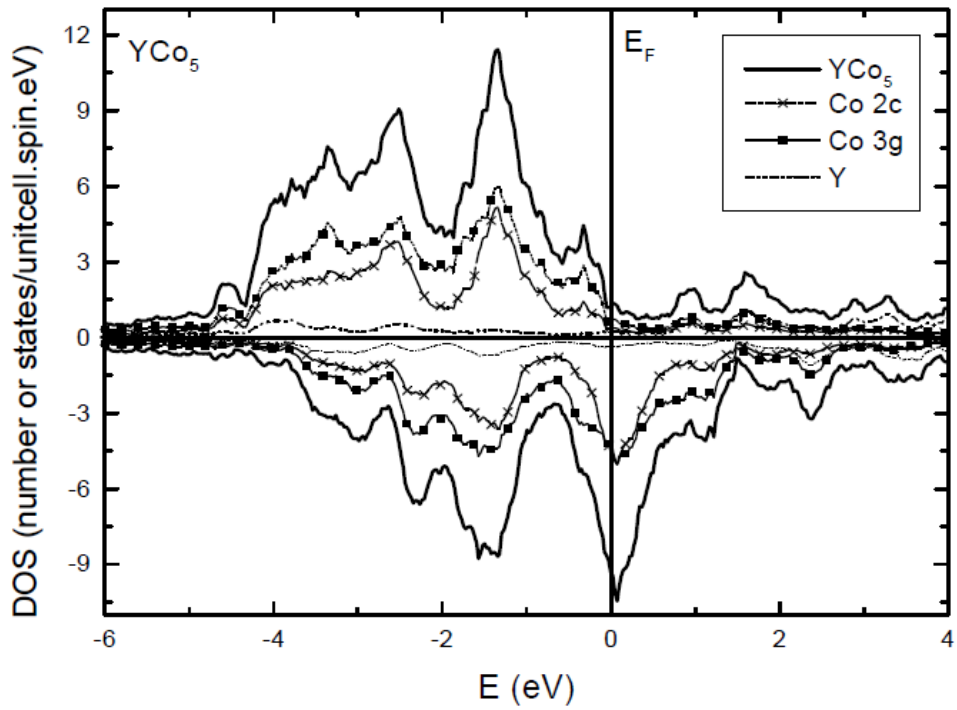

Fig. 2. Total and partial density of states of the compound YCo_5 obtained with ASW

Table 2 shows total and local spin magnetic moments calculated for the compound YCo5. In table 2 calculations reported by other authors as well as experimental values are displayed for comparison. As shown in table 2, despite the fact that pure metallic Y is non-magnetic as established above, however it has a small negative contribution to the total magnetization into the compound YCo5. It can also be observed that the biggest contribution to the magnetization of the YCo5 compound comes from Co atoms in 3g sites.

Table 2. Local and total spin magnetic moments of the compound YCo_5.

Sites	Calculated by ASW [μ_B]	Theoretical [μ_B]			Experimental [μ_B]
Y (1a)	-0.3	-0.4[29]	-0.18[1]		
Co (3g)	1.39	1.57[29]	1.52[1]	1.36[7]	1.44[30]
Co (2c)	1.49	1.68[29]	1.47[1]	1.54[7]	1.31[30]
YCo_5	6.85	7.67	7.32	7.16	6.94

Fig. 3 shows sections of the calculated spin-up and spin-down energy bands in important directions of the reciprocal lattice first Brillouin zone for the YCo_5 compound. The splitting shown for spin-up and spin-down energy bands has its origin in exchange interactions and it is congruent with the existence of ferromagnetism in this compound.

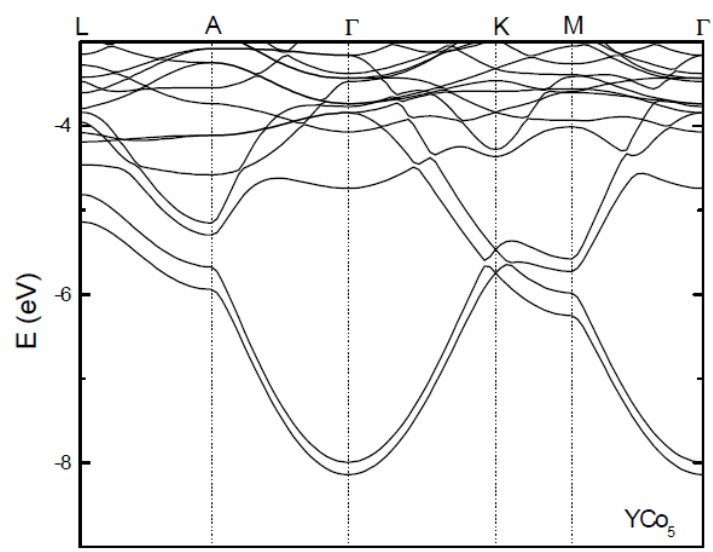

Fig. 3. Spin up and spin down energy bands of the compound YCo_5.

To simulate the application of a pressure on the YCo_5 compound, the δ parameter was varied causing, in turn, a variation in the lattice parameter of the

compound. The main results are shown in Table 3. It was observed an interesting dependence of the local moments with the lattice parameter (different simulated pressures): a bigger lattice parameter caused an increment of the magnetic moment, but a smaller lattice parameter caused a decrease in the magnetic moment until a point were there is an abrupted fall to zero (around 8.81 atomic units) and the compound suffers a magnetic phase transition from strong ferromagnetic to paramagnetic.

Table 3. Variation of the partial and total magnetization and the total energy with the latti parameter in the compound YCo_5.

δ	a (a.u.)	E_F (eV)	Magnetic moment (μ_B)				Total Energy (Ry)
			Y (1a)	Co (2c)	Co (3g)	Total	
-0.50	10.21	7.13	-0.51	3.52	4.83	7.85	-20673.26
-0.05	9.36	8.98	-0.32	3.06	4.26	7.01	-20673.62
0.00	9.26	9.27	-0.30	2.98	4.17	6.85	-20673.65
0.05	9.15	9.59	-0.28	2.87	4.04	6.63	-20673.66
0.10	9.04	9.94	-0.20	2.20	3.04	5.03	-20673.67
0.20	8.82	10.62	-0.05	1.22	0.87	2.05	-20673.67
0.20078	8.81	10.61	0	0	0	0	-20673.67
0.30	8.57	11.72	0	0	0	0	-20673.57
0.50	8.05	15.43	0	0	0	0	-20673.20

Fig. 4 shows the contributions of the (s+p) and d spin-up electrons to the total density of states of the $Y(Co,Fe)_5$ compound . As the Fe content increases the Fermi level gradually moves to the left of the density of states because Fe has lower amount of 3d electrons contributing to the band. It is also observed that the contribution of the (s+p) electrons to the density of state is much smaller than that of 3d electrons

Conclusion

Metallic Co has a magnetic moment of 1.53 μ_B and metallic Y is paramagnetic. However inside the compound YCo_5 the Y atom has a contribution to the total magnetic moment of –0.3 μ_B. Cobalt atoms in the compound YCo_5 occupy two non equivalent sites, 2c and 3g, with a contribution to the total magnetization of 1.49 μ_B and 1.39 μ_B per atom respectively. The total magnetic moment of the compound YCo_5 is 6.85 μ_B which is close to the experimental results.

A negative pressure applied to the unit cell of the compound YCo_5 caused an increase of the lattice parameter and therefore an increase in the total magnetic moment of the compound. A positive pressure cause a decrease of the magnetic moment until a sudden drop to zero occur at the lattice parameter value of 0.20078 atomic units. The substitution of Co atoms by Fe atoms in the compound $Y(Co,Fe)_5$ causes a raise in the total magnetic moment and the maximum value was found to be 9.60 μ_B for the compound YCo_2Fe_3 and then it was a slightly drop in the total magnetic moment when there is a total substitution of Co atoms by Fe atoms.

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