THE MAGNETIC MAP OF NiMn ALLOY THIN FILMS
ON Co(001) AND Co(111)

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Abstract

Following the experimental work of Groudeva-Zotova et al. (JMMM 263 (2003) 57) where the magnetic and structural characteristics of a bi-layer NiMn-Co exchange biasing systems was investigated, density functional calculations with generalized gradient corrections were performed on \((\text{Mn}_{0.5}\text{Ni}_{0.5})_n\) ordered alloy on Co(001) and one \(\text{Mn}_{1-x}\text{Ni}_x\) monolayer on Co(111). For the \(\text{Mn}_{0.5}\text{Ni}_{0.5}\) monolayer on Co(001), magnetic moments per surface atom of 0.65 \(\mu_B\) and 3.76 \(\mu_B\) were obtained for Ni and Mn, respectively. Those magnetic moments are aligned parallel to the total moment of Co(001). A complex behavior of the Mn moment in dependance of the thickness "\(n\)" is obtained for \((\text{Mn}_{0.5}\text{Ni}_{0.5})_n\) on Co(001). Investigations on \(\text{Mn}_{1-x}\text{Ni}_x\) monolayer on Co(111) have shown that the crystallographic orientation does not modify significantly neither the magnetic moments of Mn and Ni atoms nor their ferromagnetic coupling with the Co(111) substrate.
1 Introduction

The “exchange bias” phenomena, discovered by Meiklejohn and Bean [1], is the subject of flourishing studies connected to applications in spin-valves devices. Recently much attention has been given to the studies of the magnetic coupling across a ferromagnet and an antiferromagnet, which is the key element towards the understanding of these phenomena. The interaction between an antiferromagnet and a ferromagnet results in a unidirectional anisotropy which manifests itself through a displaced hysteresis loop. The shift can be useful in controlling the magnetization in devices, such as spin valves which sense changing magnetic fields through the giant magnetoresistance effect. Magnetic reading heads based on this effect are used in magnetic disk storage. The details of the coupling are presently poorly understood [2] making it difficult to optimize performance of the effect in devices. Historically, the phenomenon was first observed in fine Co particles covered by CoO.

Recently, many works have been devoted to the interface between Co and FeMn alloys [3, 4, 5, 6, 7]. Most of the experimental studies done with magneto-optic Kerr effect (MOKE), photoemission electron microscopy (PEEM) with X-ray magnetic circular dichroism (XMCD) techniques on the Co/FeMn and Co/FeMn/Co systems have been performed on simple and polycrystalline structures, prepared by magnetron sputtering and epitaxial growth techniques. Antel et al. [3] have suggested that the FeMn spin structure is aligned parallel with the magnetic moment of the Co substrate, indicating that “spin flop” coupling is not the mechanism for exchange bias in this system. Offi et al. [4] have shown that the direction of the coupling experienced by a FM film during growth on FeMn is rapidly changing spatially, leading to small domain pattern. Also, in [5], a net magnetic moment is induced in Fe and Mn when the Co film is in contact with Fe_{0.5}Mn_{0.5}, both in the paramagnetic (PM) and the antiferromagnetic (AF) state of Fe_{0.5}Mn_{0.5}. Offi et al. [6] have shown that Mn domain images could be detected in a direction which depends on whether the net magnetic moment is parallel or antiparallel to Co and Fe. Recently, Matthes et al. [7] have confirmed the localization of the Fe polarization at the Co/FeMn interfaces. For manganese the measured XMCD signals are small and below the level of signal noise.

The NiMn/Co is another prototype of exchange bias system investigated recently by Groudeva et al. [8]. One of the most important reasons is that the data published for the MnNi system show relatively high exchange bias $H_{EB}$ values both in the ”top” and in the ”bottom” configuration [9, 10]. Magnetic and structural characteristics of this bi-layer biasing (EB) systems NiMn-Co as function of the antiferromagnetic (AFM) film deposition parameters and of the post-deposition annealing and field-cooling procedures have been taken into account [8]. The obtained magnetic characteristics was closely correlated with the crystalline structure of the as-deposited samples and with the phase transformation effects. More recently, Thamankar et al. [11] have investigated Ni rich Ni$_x$Mn$_{1-x}$ alloy films grown on Cu(100) and determined their structural and magnetic properties. These films show an improved layer-by-layer growth
compared to Ni/Cu(100).

Theoretically, calculations have been performed on thin films made of 3d transition metals (TM) in order to investigate their magnetic properties. *Ab initio* calculations done by Krüger et al. [12] on 3d transition-metals on Cu(111) and Ag(111) led to the following results: (i) the Ni ML’s are nonmagnetic both on Cu(111) and on Ag(111); (ii) in the Mn ML’s the next-nearest-neighbor interaction (NNN) exchange coupling is as large or even larger than the nearest-neighbor (NN) coupling; (iii) for Mn/Ag(111) the NN coupling is weakly ferromagnetic which leads to a complex two-rows-by-two-rows antiferromagnetic structure; (iv) for the ML’s on Cu(111), the ferromagnetic-antiferromagnetic (FM-AF) state energy difference is considerably decreased as compared to ML’s on Cu(001): this is due to the triangular lattice. Full potential linearized augmented plane wave method (FLAPW) done by Bihlmayer et al. [13] on surface alloy of Mn on the Cu(111) surface indicated that the 50% alloy will not be formed at temperatures typical for epitaxial growth. Both alloys and the Mn overlayer are unstable against wetting by Cu, but the wetting energies are small. Indeed, calculations done by Krüger et al. and Bihlmayer et al. are interesting in the framework of the triangular crystalline orientation (111).

Tight-binding linear muffin-tin orbitals (TB-LMTO) [14, 15] calculations performed by M’Passi-Mabiala et al. [16, 17] have pointed out that only density functional theory (DFT) with gradient corrections reproduces the ferromagnetic properties of Mn and Co at the Mn/Co(001) interfaces. *Ab initio* calculations done by M’Passi-Mabiala et al. [18] on Fe$_{0.5}$Mn$_{0.5}$ thin films on Co(001) and Co/FeMn/Co trilayers have recently led to a more complex behaviour of the Mn polarization. An antiferromagnetic polarization between Mn atoms in nearest neighbouring FeMn alloy planes was always obtained. Very recently, the magnetic structures and anisotropy at the compensated ferromagnetic/antiferromagnetic Co/FeMn interface were investigated by the highly precise first principles FLAPW method that incorporates intra-atomic noncollinear magnetism in order to understand the magnetic complexity involved in the spin-flop coupling and the presence of intra-atomic noncollinear magnetism [19]. The self-consistent results predict that the Fe moments in the FeMn layer reorient away from their directions in bulk FeMn so as to be parallel to the Co moment direction—a reorientation that induces an out-of-plane magnetic anisotropy.

To our knowledge, no *ab initio* calculations have been done on NiMn/Co exchange biased systems up to now. Therefore, the aim of the present work is to investigate the magnetic structure of Ni$_{0.5}$Mn$_{0.5}$ ordered alloys thin films on Co(001) and Ni$_{1-x}$Mn$_x$ ML ordered alloys on Co(111) with the GGA-PW-91 functionals [20]. The ground state of fcc Co obtained by the minimisation of the total energy versus lattice parameter is performed for this functional as in [16]. At this point we have made the following approximations: (i) the lattice parameter of Co is used also for the Ni-Mn alloy film i.e. the positions of the Ni and Mn atoms are just a continuation of the position of the Co atoms. This is clearly an approximation but not too bad because Mn, Ni and Co are nearest elements in the 3d-transition metal series; (ii) no relaxation is performed;
(iii) no geometrical optimisation is performed and no search of stabilisation through exchange of atoms between Co on one hand and Ni (or Mn) on the other hand have been calculated. Such stabilisation through Mn-Co exchange has been obtained in the case of Mn-Co interfaces [16]. However, in the present case the system studied is much more complex so that there are too many variants to check; (iv) we restrict to collinear magnetism. This may not be entirely correct because Mn bulk presents some kind of non-collinear ground state [21]. Once again it should be said that extension of such model (2 chemically different atoms) to the present system (3 chemically inequivalent atoms) remains nowadays rather untractable. From all this it should be noted that since the energies between different magnetic configurations are small, one may wonder if our approach leads to real ground state.

Section II presents a brief outline of the method used whereas section III discusses the stabilization and the magnetic map of the Ni$_{0.5}$Mn$_{0.5}$ ordered alloy on Co(001). The effects of the thickness ”n” in (Ni$_{0.5}$Mn$_{0.5}$)$_n$/Co(001) have been taken into account. Section IV is devoted to (Ni$_{1-x}$Mn$_x$)/Co(111).

2 A very brief outline of the method

The calculations are performed using a scalar relativistic version of the $k$-space TB-LMTO method [14] with atomic sphere approximation. This method is based on the density functional theory [22] as outlined before. We used for Co, the lattice parameter for the ferromagnetic phase which we obtained by minimizing the total energy of the Co fcc bulk versus lattice parameter as discussed in previous work [17] for different functionals. The overlayer system is modelled, using the repeated slab geometry [23] in which 7 layers of Co(001) and 5 to 8 layers of Co(111) surrounded by layers containing Ni and Mn atoms and separated by five layers of empty spheres. These empty spheres are sufficient to prevent interaction between slabs [23] which is controlled through vanishing dispersion in the direction perpendicular to the slab and vanishing charge in the central layer of the empty spheres. The calculations are performed using an increasing number of $k$ points until final convergence is obtained in the irreducible Brillouin Zone. This is discussed in details in the Ph. D. thesis of Meza-Aguilar [24]. The description of the MnNi ordered alloy on Co(001) needs calculations with 2 inequivalent atoms per layer and for Mn$_x$Ni$_{1-x}$ alloy on Co(111), with 0.33, 0.50 and 0.66, it needs 3 inequivalent atoms per layer. Calculations were performed for (Mn$_{0.5}$Ni$_{0.5}$)$_n$, with $n=1$ to 4, on a slab of 7 monolayers of Co(001).

3 The (Ni$_{0.5}$Mn$_{0.5}$)$_n$ ordered alloys on Co(001)

The magnetic moments and total energies for the two-dimensional 1ML-thick NiMn ordered alloy on Co(001) substrate have been reported in Table 1. All possible collinear magnetic configurations have been taken into account as inputs. The $\uparrow$ and $\downarrow$ arrows indicate that the Ni or Mn moments are parallel or antiparallel to the Co moment, respectively. In the ground state
Table 1: Results for Mn_{0.50}Ni_{0.50} on Co(001). Input magnetic configurations studied, ↑ and ↓ represent the coupling between surface and substrate atoms, ↑ the coupling is ferromagnetic and ↓ the coupling is antiferromagnetic. Magnetic moments per atom, in $\mu_B$, and differences of total energies per cell (DTEC) in mRy/cell for Mn_{0.50}Ni_{0.50}/Co(001). The ground state is noted by 0.0.

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configuration the Mn and Ni atoms are ferromagnetically aligned in the surface layer. Moreover the magnetic coupling with the Co substrate is ferromagnetic as well. Similar result was already observed by M’Passi-Mabiala et al. [18] in the case of FeMn on Co(001). The magnetic configurations with the magnetization of the Ni atoms parallel to that of the Co substrate are definitively more stable than the configurations with a Ni magnetic moment opposite to that of Co.

The values of 0.65 $\mu_B$ for the Ni magnetic moment and 3.76 $\mu_B$ for the magnetic moment of Mn, obtained for n=1 in the ground state configuration, are very similar to the bulk value of Ni and to the metastable solution for Mn. The ferromagnetic coupling between Co, Ni and Mn atoms could be explained by i) the fact that Ni and Co couples normally in a ferromagnetic behavior so that this coupling tends to align Mn atoms ferromagnetically. There are also no other Mn atoms at the nearest neighboring position so that the usual antiferromagnetic tendency found in Mn bulk structure is broken. We can point out that this ferromagnetic ground state is very singular and that the other ”ferromagnetic configurations” obtained in this paper were only metastable states i.e. Mn prefers to stay in an antiferromagnetic environment; (ii) the use of the PW functional: this is a critical point and most probably more has to be done in this direction [25].

For thicker Ni-Mn coverage (n=2–4), the magnetic moments and differences of energies for (Ni_{0.5}Mn_{0.5})_n alloy on Co(001) fcc substrate were also obtained. In Table 2 we report only the magnetic moments of the ground states. The FM coupling, at the interface with Co, remains in the thickness range from 2 to 4 whereas in Ni-Mn layers not in contact with Co non-ferromagnetic configurations are observed. More precisely, an antiferromagnetic coupling between Mn atoms is depicted. The average magnetic moment per Ni atom decreases from 0.65 to 0.07 in $\mu_B$, while
the average magnetic moment per Mn atom presents an oscillatory behavior with increasing thin film thickness. Fig. 1 shows a dramatic decrease of the average Mn magnetic moment per atom as the thickness of the Mn-Ni overlayers increases. Evidence of short-range (induced) ferromagnetism is clearly shown for Mn as found in previous calculations [17] and [18]. The FM ordering between Mn and Ni surface atoms tends to disappear when the thickness of the NiMn ordered alloy increases. Also it appears that the strong antiferromagnetic behaviour between the Mn atoms tends to kill the magnetic moments on the Ni atoms. This is somewhat in reasonable agreement with XMCD [7] results, in the case of FeMn/Co where the Mn signal looks small. No MOKE and XMCD experimental results exist of our knowledge in the case of MnNi/Co so that comparison with experiments is difficult.

## 4 Results for Ni$_{1-x}$Mn$_x$ ML on Co(111)

Groudeva et al. [8] reported XRD, TEM and MOKE results for NiMn alloys on Co(111) which allow us to perform calculations of this system as function of Mn concentration in the NiMn alloy. Converged solutions for $x = 0.33, 0.50, 0.66$ are reported in Table 3 the corresponding geometric and magnetic input configurations are explained in Figures 2 and 3. Fig. 4 shows the mean magnetic moments, for Mn and Ni versus Mn (Ni) concentrations. Each converged configuration remains similar to the input one i.e. there is no modification of the spin directions of both Ni or Mn atoms, except the magnetic configuration Mn ↑ Ni ↓ in Fig. 3 where the

<table>
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<tr>
<th>Atom</th>
<th>(a) MnNi/Co(001)</th>
<th>(b) (MnNi)$_2$/Co(001)</th>
<th>(c) (MnNi)$_3$/Co(001)</th>
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Table 2: Results for (MnNi)$_n$ on Co(001) (where $n$ is 1, 2, 3 and 4). Magnetic moments per atom, in $\mu_B$, for (Mn$_{0.5}$Ni$_{0.5}$)$_n$/Co(001). Only we show the ground state, for each value of $n$ is reported. In (a), (b), (c) and (d) we present the ground state, the magnetic moments for (MnNi)$_n$/Co(001) with $n = 1, 2, 3$ and 4, respectively.
spin direction of Ni change the direction from up to down. The ground state configurations with the magnetization of the Mn atoms parallel to that of the Co substrate are definitively more stable than the configurations with a Mn magnetic moment opposite to that of Co. In the ground state configurations the magnetic moments per atom are for Mn (Ni) 3.58 (0.54), 3.52 (0.58) and -0.19 (0.18) corresponding to $x = 0.33$, 0.50 and, 0.66, respectively. For Mn poor contents up to $x=0.50$, the FM coupling between Mn and Ni atoms remains whereas it is ferrimagnetic for Mn rich content in agreement with our previous works [17]. The magnetic moment are reduced to -0.19 and 0.18 for Mn and Ni, respectively. When we compared the magnetic moment in Mn$_{0.5}$Ni$_{0.5}$ on Ni(001), the more compact (001) surface induced a higher moment of 3.76$\mu_B$ compared to the 3.52$\mu_B$ of the Mn$_{0.5}$Ni$_{0.5}$ on Ni(111) surface, down to the metastable one value. The results mentioned above could be attributed in comparison to the (001) direction to the high coordination in the triangular lattice. Relatively, few works, however, have considered triangular ML’s on the fcc (111) surfaces, especially as far as ab–initio calculations are concerned. This somewhat surprising since one may expect the growth conditions to be equally good for both surfaces and the stability to be even higher for the triangular ML’s due to their maximal coordination of 6. The middle–of–row TM elements V, Cr, Mn tends towards antiferromagnetic nearest–neighbor coupling, which is completely frustrated on the triangular lattice [12]. Therefore noncollinear spin orders may arise and longer ranged spin couplings become important. The determination of the ground–state spin order may then be a nontrivial problem even in localized spin models. We have also to point out that our calculations did not take relaxations effect into account. According to Groudeva et al. [8] reported XRD, TEM and MOKE results, the as–deposited samples are a mixture of a non–equilibrium FCC NiMn phase and a variable amount of the equilibrium face centred tetragonal (FCT) phase.

5 Conclusion and outlook

In the present communication we investigate a MnNi/Co exchange bias system as already done for FeMn/Co by M’Passi-Mabiala et al. [18]. For this purpose we have determined the magnetic map of ”n” layers ($n = 1$ to 4) of ordered (Ni$_{0.5}$Mn$_{0.5}$)$_n$ alloys on Co(001) and one monolayer thick Ni$_{1-x}$Mn$_x$ alloys on Co(111) within the ab initio TB-LMTO method with gradient corrections. Ferromagnetic coupling between Mn and Ni is obtained in the Mn-Ni monolayer in contact with the Co(001) substrates. Moreover this coupling is also ferromagnetic between Mn, Ni and Co for interface-layers. This ferromagnetic polarization is clearly short-ranged. For the (111) crystallographic orientation, the situation is very different: although for low Mn concentration (less or equal to 0.50) the magnetic couplings remain always ferromagnetic, for $x = 0.66$ a strong antiferromagnetic coupling appears between the Mn atoms. Moreover, this antiferromagnetic coupling between the Mn atoms kills the magnetic moment on the Ni atoms. We expect that our results will give a new impetus to the experimental community to study in more details the
Table 3: Magnetic moments (in $\mu_B$) for Mn, Ni (in parenthesis) and Co, for each ground state for different geometric configurations (see Fig. 2); results (a) for Mn$_{0.33}$Ni$_{0.66}$, (b) for Mn$_{0.50}$Ni$_{0.50}$ and (c) for Mn$_{0.66}$Ni$_{0.33}$. Co4 are the atoms in the interface and Co1 are the atoms in the center of the slab.

MnNi/Co system as already done for the FeMn/Co system. [4, 5, 6, 7]. Also calculations taking into account non-collinear magnetism and the optimization of the geometry have to be done.

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References


Figure 1: Results for (Ni_{0.5}Mn_{0.5})_{n} monolayers on Co(001), "n" is the thickness of MnNi overlayers. Mean magnetic moment per atom (in $\mu_B$), for Ni and Mn atoms as a function of the MnNi thickness. Line with circles (triangles) represent the mean magnetic moment for Mn (Ni) atoms.

Figure 2: Schematic representation of the geometric configurations studied. Surface geometric configurations for Mn$_x$ Ni$_{1-x}$ monolayer alloy on Co(111) with (a) $x=0.33$, (b) $x=0.50$ and (c) $x=0.66$. Thick dashed lines represent the geometric unit cells and the solid line represent the position relative between Mn and Ni atoms. In (a) the Mn atom is surrounded by Ni atoms; in (b) the Mn and Ni atoms are aligned by lines and in (c) the Ni atom is surrounded by Mn atoms.
Figure 3: Schema of magnetic configurations studied. Input magnetic configurations studied in each case, for Mn$_x$Ni$_{1-x}$ on Co(111), (a) $x=0.33$, (b) $x=0.50$ and (c) $x=0.66$. The empty (filled) circles are the Ni (Mn) atoms. The up (down) arrow represent the ferromagnetic (antiferromagnetic) coupling between Co substrate atoms. Thick dashed lines represent the magnetic unit cells and the solid line represent the position relative between Mn and Ni atoms.
Figure 4: Results for Mn$_x$Ni$_{1-x}$ monolayer on Co(111) substrate. Mean magnetic moment (in $\mu_B$) for Mn and Ni atoms versus Mn concentration (where $x=0.33, 0.50, 0.66$). Line with squares (diamonds) represent the mean magnetic moment for Mn (Ni) atoms.