ELSEVIER

Computational Materials Science 10 (1998) 245–248

COMPUTATIONAL MATERIALS SCIENCE

Non-collinear magnetism and exchange couplings in FeCo/Mn superlattices

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Abstract

We present the main results of a systematic study of the magnetic properties of Fe_xCo_{1-x}/Mn_n for various Fe concentrations x and Mn thicknesses n. We show that the magnetic order in the Mn spacer changes from collinear to non-collinear when the Fe concentration decreases. This behaviour is discussed in relation with a bulk 'canted' magnetic state nearly degenerate with the collinear AF order. The origin of the exchange of stability between these two magnetic states is ascribed to a stronger collinear character of the Fe/Mn interface than the Co/Mn one. © 1998 Elsevier Science B.V.

Keywords: Non-collinear magnetism; Metallic superlattices; Interlayer couplings

1. Introduction

It has been shown recently that FeCo/Mn multilayers present very interesting magnetic properties related to non-collinear orders in the Mn spacer. First, a large biquadratic coupling has been obtained [1] and it has been shown that the coupling energy follows the Slonczewski parabolic law [2]. Second, a net magnetic contribution of the antiferromagnetic Mn spacer has been found [3,4] which makes an angle of 23° with the total FeCo magnetization. These properties have been ascribed to interfacial roughness [2]. However, the used models are based on micromagnetism approaches. The aim of the present work is to study these systems from the electronic structure viewpoint.

Such a complete electronic structure study of Fe_xCo_{1-x}/Mn_n superlattices is under progress since more than two years in our group within the tight binding framework using the real space recursion technique [5–7]. We have developed a new code for massively parallel computers in order to determine self consistently the magnetic moments vectors distribution in superlattices. The method and technical details are given in two other papers in these proceedings [8,9]. In this paper, we present a summary of the latest achievements of this study. We show that the magnetic behaviour of thin Mn spacers is highly sensitive to the Fe concentration of the FeCo ferromagnetic layer: from collinear antiferromagnetic for pure Fe, it becomes non-collinear for pure Co. This result is discussed in relation with bulk 'canted' states and interfacial non-collinear character of the Mn.

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PII S0927-0256(97)00148-1

2. Non-collinear magnetic behaviour of the Mn spacer

A preliminar study of the bulk Mn [8,9] has shown that the antiferromagnetic (AF) collinear order is the most stable state as compared to helicoidal or spin spiral magnetic configurations. However, it as been pointed out that a 'canted' state corresponding to a spin spiral with the direction of the magnetic moments in the i-th plane equal to $\theta_i = \theta \cong 0.4\pi$ and $\varphi_i = i \cdot \pi$ is nearly degenerate with the AF order. In the case of superlattices under study in this paper, where the angular degree of freedom is restricted to θ ($\varphi_i = 0$), this 'canted' state plays an important role. Indeed, it corresponds to the magnetic configuration which is the most similar to the AF one when all magnetic moments are in the (xOz) plane. However, the energy difference of approximately 1 meV/atom between both states should give collinear ground states for the superlattices.

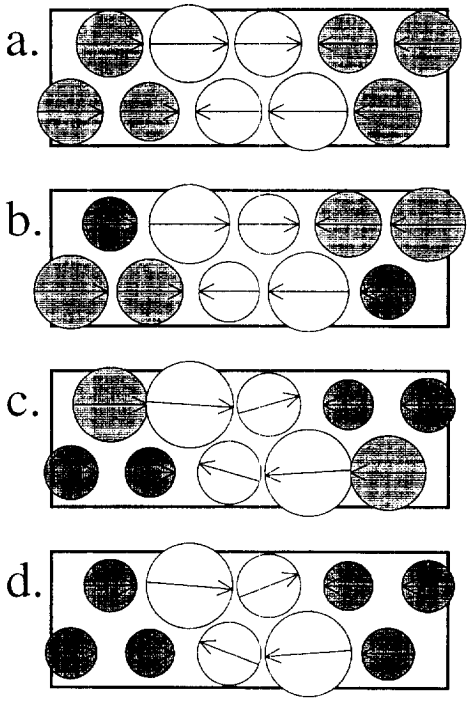

Fig. 1. Magnetic moments distributions for Fe_xCo_{1-x}/Mn_4 superlattices for (a) $x = 1$, (b) $x = 1/2$ with a pure Fe monolayer at the interface, (c) $x = 1/2$ with a pure Co monolayer at the interface and (d) $x = 0$. Each magnetic moment is represented by an arrow giving its direction and the diameter of the circle is equal to its length. The Mn are in white, the Co atoms in dark grey and the Fe atoms in light grey. Only the magnetic moments on the atoms in the unit cell are shown.

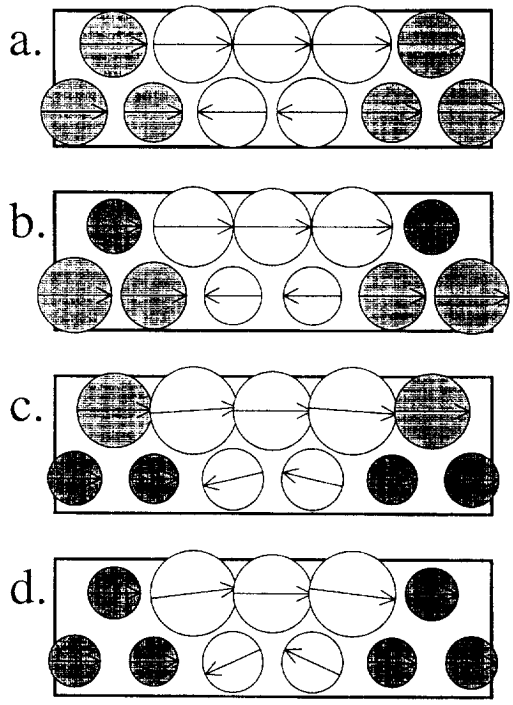

Fig. 2. Magnetic moments distributions for Fe_xCo_{1-x}/Mn_5 superlattices for (a) $x = 1$, (b) $x = 1/2$ with a pure Fe monolayer at the interface, (c) $x = 1/2$ with a pure Co monolayer at the interface and (d) $x = 0$. Each magnetic moment is represented by an arrow giving its direction and the diameter of the circle is equal to its length. The Mn are in white, the Co atoms in dark grey and the Fe atoms in light grey. Only the magnetic moments on the atoms in the unit cell are shown.

Surprisingly, the ground state in not always collinear depending on the Fe concentration of the FeCo ferromagnetic layers. Figs. 1 and 2 show the magnetic moments distributions for Fe_xCo_{1-x}/Mn_4 and Fe_xCo_{1-x}/Mn_5 superlattices for the expected ground state i.e. for an antiferromagnetic interlayer arrangement when $n = 4$ and for a ferromagnetic interlayer arrangement when $n = 5$. For a pure Fe ferromagnetic layer (Fig. 1a and Fig. 2a) or for $x = 1/2$ with a pure Fe interfacial monolayer (Fig. 1b and Fig. 2b), the magnetic order is obtained collinear. The coupling between the Fe and Mn interfacial magnetic moments is parallel and the Mn moments of the second atomic layer from the interface are reduced as compared to the others in agreement with ab initio calculations of these collinear

states [5–7]. For $x = 1/2$ with a pure Co interfacial monolayer (Fig. 1c and Fig. 2c) or for a pure Co ferromagnetic layer (Fig. 1d and Fig. 2d), two solutions are obtained: the collinear one with very similar magnetic moments distributions as for the two previous cases and a non-collinear one shown by the figures. For $n = 4$ (Fig. 1), the canted character of the non-collinear state in the Mn spacer can be clearly seen mainly on the two inner atomic layers. This state is less pronounced for $n = 5$ (Fig. 2) where the inner Mn magnetic moments is exactly collinear with the ferromagnetic moments by symmetry.

3. Interlayer coupling energy

We have calculated the total energy as a function of the angle $\Delta\theta$ between the inner magnetic moments (whose directions are fixed) of successive FeCo layers. This allows the determination of the interlayer magnetic couplings between the FeCo layers through the Mn spacer as a function of $\Delta\theta$ when the Fe concentration and the Mn thicknesses vary. This situation is similar to the case where an external magnetic field is applied maintaining the relative angle $\Delta\theta$ constant. The results are reported in Fig. 3 for the same four cases as for Figs. 1 and 2. The energy curves are very similar and roughly follow parabolic laws. However, for pure ferromagnetic layers, the energy variations are approximately two times smaller than the ones obtained for FeCo alloys. They are, for these alloys, nearly the same whatever the element at the interface is. For $x = 1$ and $x = 1/2$ with a pure Fe interfacial monolayer, the energy is the lowest for $\Delta\theta = 180°$ when $n = 4$ and for $\Delta\theta = 0°$ when $n = 5$. For $x = 1/2$ with a pure Co interfacial monolayer, the collinear solution is nearly degenerate in energy with the non-collinear states presented in Figs. 1 and 2. However, only the collinear solution is stable from the angular viewpoint. For $x = 0$ (pure Co ferromagnetic layer), the energy minimum is obtained for $\Delta\theta \cong 150°$ when $n = 4$ and for $\Delta\theta \cong 25°$ when $n = 5$. However, as mentioned previously [8,9], these minima do not correspond to angular stable solutions because the perpendicular compo-

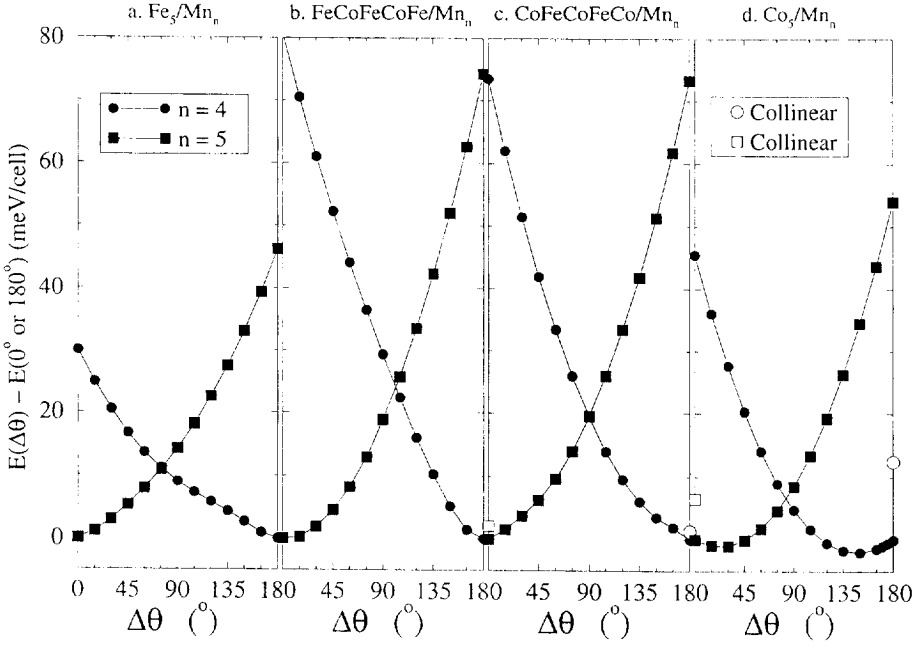

Fig. 3. Total energy of Fe_xCo_{1-x}/Mn_n superlattices as a function of $\Delta\theta$ ($n = 4$ circles and $n = 5$ squares) for (a) $x = 1$, (b) $x = 1/2$ with a pure Fe monolayer at the interface, (c) $x = 1/2$ with a pure Co monolayer at the interface and (d) $x = 0$. The energy of the collinear situation are given by the open symbols.

nent $M_{d,\theta}$ on the sites for which the angles are fixed is not equal to zero. As a consequence, the angular stable states correspond to $\Delta\theta \cong 175°$ when $n = 4$ and to $\Delta\theta \cong 3°$ when $n = 5$. Finally, these states are clearly more stable than the collinear solution with a surprising large difference (more than 12 meV per cell corresponding to 3 meV per Mn atom when $n = 4$).

4. Discussion

To summarise, we have shown that for $x = 1$ and $x = 1/2$, the most stable state is obtained for $\Delta\theta = 180°$ when $n = 4$ and for $\Delta\theta = 0°$ when $n = 5$ and is collinear (even if other solutions are obtained for $x = 1/2$ with a pure Co interfacial monolayer presenting non-collinear Mn configurations). We have also shown that for $x = 0$, the most stable state corresponds to $\Delta\theta \cong 175°$ when $n = 4$ and to $\Delta\theta \cong 3°$ when $n = 5$ with a significant non-collinear order in the Mn spacer. This result can be qualitatively understood from the existence of a bulk 'canted' state nearly degenerate with the AF order. However, it is not clear why this new state becomes the most stable when the Co concentration increases. This point is under study and will be discussed in detail in a forthcoming paper.

At the present status of our work, we can give two possible origins for this stability exchange between AF collinear and 'canted' non-collinear states: (i) a consequence of the thin thickness of the film, for which the magnetic behaviour of the Mn spacer is completely different from the one for large films or bulk and, (ii) an interfacial origin resulting from different Co/Mn and Fe/Mn interfacial couplings. It seems that both contribute: the first allows the 'canted' state to exist when the interfacial coupling does not tend to destroy it. This is illustrated by Fig. 4 showing the magnetic moments distributions for FeCoFeCoFe/Mn_{20} and for CoFeCoFeCo/Mn_{20} superlattices with $\Delta\theta = 180°$. We see clearly that the two magnetic configurations are very similar in the centre of the Mn layer whereas near the interfaces they are completely different: for FeCoFeCoFe/Mn_{20}, the two first Mn monolayers present a nearly collinear magnetic configuration. This shows that the Fe/Mn interface presents a higher level of collinearity than the Co/Mn one. This point will be extensively studied in the future.

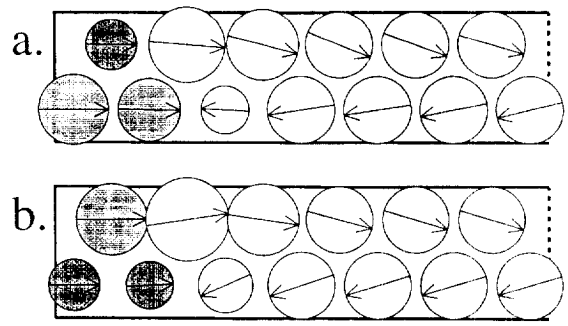

Fig. 4. Magnetic moments distributions for $Fe_{0.5}Co_{0.5}/Mn_{20}$ superlattices for (a) a pure Fe monolayer at the interface, (b) a pure Co monolayer at the interface. Each magnetic moment is represented by an arrow giving its direction and the diameter of the circle is equal to its length. The Mn are in white, the Co atoms in dark grey and the Fe atoms in light grey. Only the magnetic moments on the atoms in half of the unit cell are shown.

Acknowledgements

The calculations have been mainly realised on the T3E parallel computer of the Institut du Développement et des Ressources en Informatique Scientifique (IDRIS) of the CNRS and on the SP2 parallel computer of the Centre National Universitaire Sud de Calcul (CNUSC).

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