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Magnetic structure of fcc Fe films on Co(1 1 1)

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Abstract

The collinear magnetic structure of n ($n = 1, \ldots, 6$) monolayers (ML) of Fe films deposited on Co(1 1 1) substrate is investigated by ab initio density functional theory within a generalized gradient approximation. We have found that the ferromagnetic ground state exists only for one Fe monolayer. For higher thickness, a sequence of antiferromagnetic coupling with low magnetic moments in the inner layers of films is identified as ground state.

Keywords: Magnetic structure; fcc Fe films; Co substrate

1. Introduction

The strong correlation between structural and magnetic properties of face centred cubic (fcc) Fe films deposited on copper substrate with different crystallographic orientations and on cobalt with (1 0 0) direction, have been the subject of extensive researches. Several experimental techniques such X-ray magnetic circular dichroism (XMCD) [1], magneto-optic Kerr effect (MOKE) [2] and photoemission [3] have been extensively used for the exploration of the magnetism and structural details of fcc Fe films, in particular their dependence on the Fe film thickness. On Cu(1 0 0), Fe films assume a ferromagnetic (FM) face centred tetragonal (fct) structure for thickness below 4 monolayers (ML) (region I) and an antiferromagnetic (AFM) fcc structure at thickness between 5 and 11 ML (region II). For these thicknesses, the stabilization of this structure is due to the expansion of interlayer distances between ferromagnetically coupled layers and a contraction of distances for antiferromagnetically coupled layers [4]. Fe films thicker than 11 ML transform in FM body centred cubic (bcc) phase (region III) [1,2,5]. Comparing reflexion high-energy diffraction (RHEED) oscillations results and magnetic measurement by MOKE technique, Escrocia-Aparicio et al. [2] have observed the same structural and magnetic behaviors in Fe/Co(1 0 0) than those of Fe/Cu(1 0 0) with small difference in magnetic moments due to substrate polarization. By XMCD technique, Schmitz et al. [5] have found that the Fe spin moment is 3 μ_B on Co(1 0 0) and 2.8 μ_B on Cu(1 0 0) in region I. In region II, it decreases to 1.1 and 0.8 μ_B for Fe/Co(1 0 0) and Fe/Cu(1 0 0), respectively. For a Fe thickness larger than 10 monolayers, the magnetic moment in the Fe coverage increases again.

From theoretical studies [4,6], Asada and Blügel [6] have investigated the collinear magnetism of n ($n = 1, \ldots, 6$) monolayers of Fe films deposited on Cu(1 0 0) using full-potential linearized augmented plane-wave (FLAPW) method. They have found that FM order is the ground state up to 3 ML, whereas above this thickness, Fe films present a bilayer AFM coupling for an even number of monolayers, and a sequence of several spin states for an odd number. Therefore, the magnetic transition from the FM to the AFM states occurs for $n = 3$ ML, whereas the experimental result [5] predicts a magnetic transition for $n = 4$ ML. This discrepancy can be explained by the perfect interface considered in theoretical studies. Indeed, in experimental investigations, such perfect interfaces do not exist, because the Fe films growth is accompanied by the apparition of roughness, interdiffusion effects and complex reconstructions at the interface [7,8] which have a strong influence on the magnetism and structure of Fe films [9–11]. Those effects lead to the formation of spin spiral density wave [12–20].

In order to provide additional information about electronic effects of the substrate nature on the magnetic phases of fcc Fe

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films, the magnetic structure of Fe/Co(1 0 0) system has also been studied using ab initio calculations. Using tight binding linear muffin-tin orbital with atomic sphere approximation (TB-LMTO-ASA) method within local spin density approximation (LSDA), Mokrani et al. [21] have found that the Fe films are ferromagnetic only for one and two monolayers. However, because the LSDA does not give the correct Fe magnetic ground state [22], Spišák and Hafner [23] have used ab initio local spin density technique including generalized gradient corrections (GGC) to investigate Fe/Co(1 0 0) magnetism. Up to three monolayers, they have found similar results than those of Mokrani et al. [21] with however a considerable difference in the magnetic moments and energy differences. In addition, they have found that above 3 ML, Fe films produce a bilayer AFM ground state for an even number of Fe layers, while for an odd number, several spin structures coexist. The failure to predict ferromagnetism in Fe films with three and four monolayers as observed experimentally has been attributed to the influence of the epitaxial constraint of Co/Cu(1 0 0) on the magnetism of Fe films since the fcc structure of Co is stabilized by epitaxial growth on Cu(1 0 0) [1]. Another factor that could affect the magnetism of fcc Fe films is the intermixing Fe–Co at the interface since Co and Fe show a large mutual solubility.

Today, interest is focused on growth and magnetism of fcc Fe films on Cu(1 1 1) surface. Experimentally, it was shown that, by using thermal deposition (TD), Fe films on Cu(1 1 1) undergo a transition from fcc low-spin (LS) to bcc high-spin (HS) ferromagnetic states for three monolayers [24], while by pulse laser deposition (PLD), an isomorphic fcc Fe is stabilized up to six monolayers [25,26]. The oscillations of total magnetic moment as a function of film thickness have been determined by MOKE technique [25], where it was observed that magnetic phase transformation from HS-FM to LS-FM order occurs at a thickness of about three monolayers. The article of Shen et al. [27] gives a description of the structure, morphology and magnetism of ultrathin Fe films epitaxially grown on Cu(1 1 1) surface. However, very few calculations have been devoted to magnetic and structural properties of those systems. In their study of magnetism of transition metals on Cu(1 1 1) and Ag(1 1 1) substrates, Krüger et al. [28] have found ferromagnetic order as ground state for 1 ML of Fe/Cu(1 1 1). In addition, Krüger [29] has studied the collinear magnetism of Fe films deposited on Cu(1 1 1) for thickness up to six monolayers using TB-LMTO-ASA based on both GGA and LSDA approximations. This author found that for the GGA approach, the ground state is ferromagnetic up to 3 ML while this FM coupling is stable only for 2 ML for the LSDA approximation. Comparing magnetic behavior of Fe films as function of their thickness with experimental data, he found similar oscillatory behavior. He attributed this spin transition to a competition between surface/interface effects and preferentially ferromagnetic coupling between adjacent monolayers on one hand and bulk like spin-density wave correlations on the other hand. In their recent study, Spišák and Hafner [30] have proved that as for Fe/Cu(1 0 0), the magnetism of fcc Fe films on Cu(1 1 1) is strongly coupled to structure distortions.

In the literature, several attempts have been made to study the magnetic behavior of Fe films deposited on Cu(1 0 0), Co(1 0 0) and Cu(1 1 1) substrates, but, until now, there are no theoretical nor experimental investigations on the magnetic structure of Fe/Co(1 1 1). As it is well known, the magnetic properties of ultrathin films depend on the details of atomic structure, it is therefore, worthwhile to determine the magnetic behavior of fcc Fe films on Co(1 1 1) and compare it with [1 0 0] direction in order to understand the effect of symmetry and coordinations number change. This aspect constitute the first aim of our study. The second motivation of this work is to compare the general trends and to highlight both common and distinct properties obtained for Fe/Co(1 1 1) with those of Fe/Cu(1 1 1) system.

The rest of this paper is organized as follows: After a brief account in Section 2 of the theoretical model used for calculations in the framework of the TB-LMTO-ASA method, the results of the magnetic map of Fe/Co(1 1 1) are presented and discussed in Section 3. The main conclusions of the study are summarized in the last section.

2. A brief outline of the method

The collinear magnetic calculations of Fe films on Co(1 1 1) are performed using a scalar-relativistic version of the *k*-space tight binding linear muffin-tin orbitals with atomic sphere approximation (TB-LMTO-ASA) method [31,32]. Since the LSDA approach cannot give the correct ground state of ferromagnetic bcc Fe [4,22,33], we have used the generalized gradient approximation with Langreth-Mehl-Hu functional (GGA-LMH) [34]. Several studies have been done for magnetic properties of bulk fcc Fe [35,36] and they have shown that its magnetic ground state is AFM with an equilibrium lattice parameter of 6.56 a.u. and magnetic moment of 1.0 μ_B. This lattice parameter is used in our study. The choice of GGA-LMH [34] approximation is also a result of our calculations of equilibrium lattice parameter of fcc Co in bulk. As shown in Table 1, the lattice constant of fcc Co (a = 6.63 a.u.) and magnetic moment (μ = 1.63 μ_B) obtained from the GGA-LMH are in good agreement with experimental parameter (a = 6.68 a.u., μ = 1.61 μ_B) [37] and with previous calculation Spišák and Hafner [23] (a = 6.64 a.u). In order to investigate magnetic properties of Fe films, we have used the super-cell technique. Since the experimental studies [41]

Table 1
Lattice parameter (in a.u.) of Co bulk calculated with LSDA of Vosko-Wilk-Nusar (VWN) [38] and von Barth-Hedin (v.BH) [39] functional and with GGA of Perdew-Wang (PW91) [40] and Lagnreth-Mehl-Hu(LMH)[34] functional compared to the experimental one [37]

Exchange-correlation functional	LSDA		GGA		Exp.
	vBH	VWN	LMH	PW91	
Lattice parameter Co(fcc) (a.u.)	6.55	6.56	6.63	6.80	6.68
Magnetic moment (μ_B/atom)	1.57	1.62	1.63	1.69	1.61

have shown that the fcc structure of Co is stabilized on Cu(1 1 1) up to 6 ML and above this thickness Co transforms to the hcp structure, we have represented Fe/Co(1 1 1) system by five Co substrate layers. It is also important to notice that for this number, the Co central layer properties coincide with those of the bulk. A variable number n ($n = 1, \ldots, 6$) of Fe layers are deposited on both sides of Co followed by five layers of empty spheres to represent vacuum space. This number of vacuum layers is sufficient to cancel any interaction between two consecutive *slabs*. In our study, the Fe films are assumed to grow pseudomorphically on Co(1 1 1), i.e., the Fe films adopt the lateral spacing of Co, whereas, the inter-layer distances Fe–Fe are calculated according to the constant volume approximation. For the k integration, we have used 64 k points in the two dimensional irreducible Brillouin zone.

3. Magnetic structure of Fe/Co(1 1 1)

3.1. Results

For one Fe monolayer ($n = 1$ ML) on Co(1 1 1), we have considered three magnetic solutions: p(1 × 1)↑ and p(1 × 1)↓ corresponding to the in-plane ferromagnetically ordered layers, where the Fe magnetic moments are respectively parallel and antiparallel to Co moments and an in-plane antiferromagnetic order c(2 × 2). We found that the p(1 × 1)↑ is clearly the ground state. The metastable solutions p(1 × 1)↓ and c(2 × 2) are about 50 meV/atom higher in energy. The Fe monolayer exhibits a larger magnetic moment (2.51 μ_B) in p(1 × 1)↑ solution compared to p(1 × 1)↓ case (−2.42 μ_B). The Co interface magnetic moment of the ground state configuration (1.53 μ_B) is reduced as compared to the Co central layer (1.68 μ_B). A very drastic decrease of the Co magnetic moment in the metastable solution case (0.01 μ_B) is found. This decrease is due to the strong Fe–Co antiferromagnetic coupling at the interface.

Since we have found that for 1 ML Fe on Co(1 1 1) the c(2 × 2) magnetic configuration is largely higher in energy, we can discard it and restrict the calculations to the simple p(1 × 1) unit cell for thicker films. For $n \geq 2$ ML, we have considered 2^n magnetic configurations in which, in most cases, the input ferromagnetic configurations are unstable since they converge to an antiferromagnetic order during the self-consistent process. The magnetic moments of the ground and metastable states of Fe on Co(1 1 1) are listed in Table 2 together with the interface magnetic moments of Co. The ↑(↓) notation refers to Fe plane when the magnetic moment orientation is parallel (antiparallel) to that of the substrate, going from the interface to the surface.

For 2 ML, we have examined all possible magnetic configurations within the p(1 × 1) unit cell. We have found only two converged magnetic solutions: ↑↓ and ↑↑. The ↑↓ solution is energetically more favourable by 18.79 meV/atom. One can notice that this value is very small compared to that found in the case of 1 Fe ML (50 meV/atom). The surface effect enhances the magnetic moment of Fe at the surface compared to the bulk Fe magnetic moment in the case of the two solutions, but this enhancement is less important in the case of AFM coupling. Also, in the magnetic ground state, the Fe surface magnetic moment is 42% higher than the subsurface magnetic moment.

For 3 ML, the ↑↑↑ order is found numerically unstable and converged to ↑↓↑ order after self-consistent iterations. Indeed, among the 2^3 configurations investigated, we have obtained only two converged magnetic solutions: ↑↑↓ and ↑↓↑. As displayed in Table 2, the ↑↑↓ solution is shown to be the ground state. The metastable solution is 5.78 meV/atom higher in energy. A very low magnetic moment (0.21 μ_B) is found at the subsurface while this moment is −1.86 μ_B at the surface.

For a film consisting of 4 Fe ML, two magnetic solutions are again found: ↑↓↓↑ and ↑↓↓↓. The calculated ground state configuration is ↑↓↓↑ with an energy difference of 5.81 meV/atom. The surface, subsurface and interface magnetic moments ground state are 1.98, −0.21 and 1.42 μ_B, respectively.

For 5 Fe ML, all input magnetic configurations have converged to ↑↓↑↑↓ and ↑↓↓↑↑ solutions, where, the former is identified as the ground state. It is about 5.1 meV/atom lower in energy than the second solution. The magnetic moment in the inner layers decreases from interface to subsurface:

Table 2
Energy difference ΔE of n ($n = 1, \ldots, 6$) monolayers of Fe on Co(1 1 1) between magnetic solutions in meV/atom, magnetic moment of Co at interface ($\mu_{Co(I)}$) total magnetic moments μ_{film} (μ_B) and the local magnetic moments μ_i (μ_B)

Fe coverage	Magnetic states	ΔE	μ_{film} (μ_B)	$\mu_{Co(I)}$	μ_1	μ_2	μ_3	μ_4	μ_5	μ_6
$n = 1$ ML	↑	00	2.51	1.53	2.51					
	↓	50.21	−2.42	0.01	−2.42					
$n = 2$ ML	↑↓	00	−0.83	1.60	1.16	−1.99				
	↑↑	18.79	4.49	1.70	2.13	2.35				
$n = 3$ ML	↑↑↓	00	0.21	1.68	1.86	0.21	−1.86			
	↑↓↑	5.78	3.14	1.61	1.39	−0.36	2.11			
$n = 4$ ML	↑↓↓↑	00	2.14	1.60	1.42	−1.05	−0.21	1.98		
	↑↓↓↓	5.81	−1.69	1.59	1.37	−0.86	−0.25	−1.95		
$n = 5$ ML	↑↓↑↑↓	00	−0.73	1.59	1.33	−1.16	0.75	0.34	−1.99	
	↑↓↓↑↑	5.10	2.98	1.62	1.47	−0.25	−0.42	0.22	1.96	
$n = 6$ ML	↑↓↑↓↓↑	00	2.07	1.59	1.36	−0.98	0.61	−0.68	−0.22	1.99
	↑↓↓↑↑↓	0.80	−0.54	1.62	1.50	−0.59	−0.66	1.01	0.15	−1.95

The ↑(↓) notation refer to Fe ML when the magnetic moment orientation is parallel (antiparallel) to that of the substrate going from interface to the surface.

$\mu_1 = 1.33\ \mu_B$, $\mu_2 = -1.16\ \mu_B$, $\mu_3 = 0.75\ \mu_B$, $\mu_4 = 0.34\ \mu_B$ in the case of the ground state. However, due to the reduced number of neighbours atoms at the surface, the Fe surface magnetic moment is increased ($-1.99\ \mu_B$). Note that the Fe quenched magnetic moment at the interface is a consequence of its antiferromagnetic coupling with adjacent Fe layer.

As for 5 ML, Fe film with 6 ML develops a sequence of antiferromagnetic coupling defined by two magnetic solutions nearly degenerate: ↑↓↑↓↓↑ and ↑↓↓↑↑↓. The first solution is lowest in energy by 0.8 meV/atom. The magnetic solutions are characterized by large surface magnetic moment compared to those of inner layers. In fact, inside Fe films, the magnetic moments are very low, consequence of antiferromagnetic coupling between adjacent layers.

3.2. Discussion

Our results concerning the magnetic ground state of Fe films grown on fcc Co(1 1 1) may be summarized as follows: (i) The ferromagnetic order appears only for 1 ML. (ii) The interfacial Fe/Co coupling is always ferromagnetic. The Fe magnetic moments values are reduced at the interface due to the antiferromagnetic coupling with adjacent Fe layer. (iii) For all Fe film coverages, the surface and subsurface coupling is always antiferromagnetic. (iv) The coordination number reduction favours a relatively high surface magnetic moment which is of about 2 μ_B for $n > 1$ ML. Thus, these values are almost independent of coverage and ground state spin order. (v) The subsurface magnetic moments are drastically reduced (except for 1 ML) and they are almost independent of coverage. (vi) The antiferromagnetic coupling between Fe adjacent inner layers leads to a strong decrease of the local magnetic moments. (vii) For $n \geq 3$, the converged magnetic solutions are almost degenerated. In general, the magnetic energy difference decreases whenever the Fe film thickness is increased (Fig. 1a)

As it is well known, the magnetic behavior of ultrathin films depends strongly on the crystallographic orientations, it is therefore, interesting to compare the magnetic structure of fcc Fe on Co(1 1 1) surface with Fe/Co(1 0 0). Analyzing the results of Fe/Co(1 0 0) given by Spišák and Hafner [23] and comparing them with our results, we found that for both systems, the surface magnetic moments are enhanced, while a strong decrease of magnetic moments is observed in the inner layers due to the antiferromagnetic coupling between Fe adjacent layers which favours the onset of small magnetic moments. It is important to notice the existence of a considerable difference in calculated Fe magnetic moments between these two surfaces: for 1 ML of Fe/Co(1 0 0), the magnetic moment is more larger (2.77 μ_B) than the (1 1 1) surface one's (2.51 μ_B). This enhancement can be attributed to the reduction of the local coordination number at the (1 0 0) surface compared to (1 1 1) surface. Another common feature is observed at the interface where the magnetic coupling between Fe and Co, in both cases, is always ferromagnetic and the Fe–Co interaction reduces the interface Co magnetic moment.

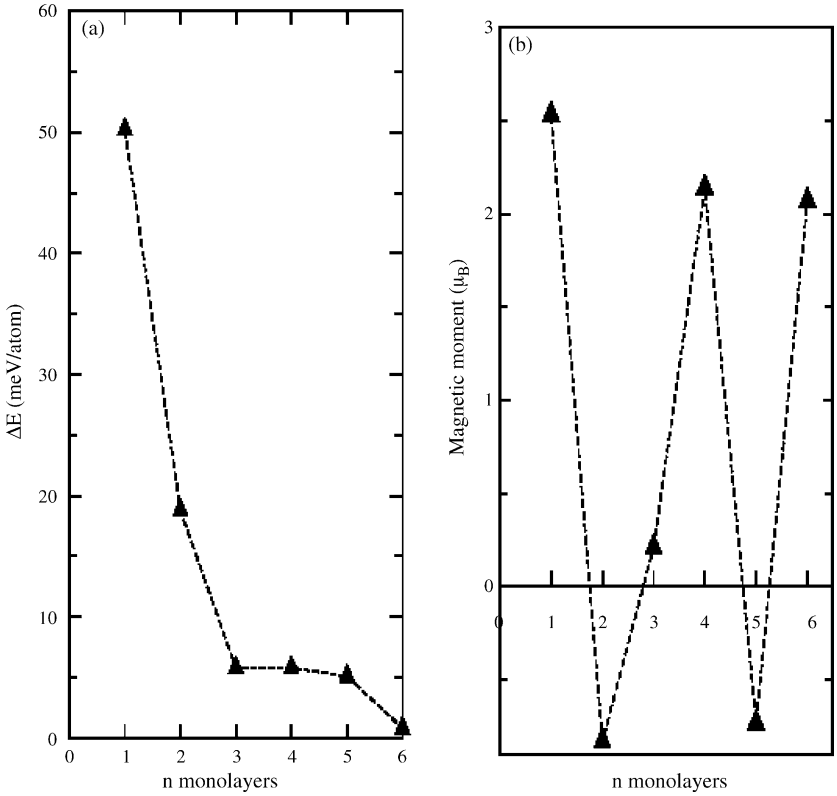

Fig. 1. (a)Variation of energy magnetic difference between the ground and metastable states (in meV/atom) with Fe films coverages. (b) Variation of the total magnetic moment (in μ_B) of the Fe films coverages.

From an energetic point of view, the stabilized magnetic configurations are very different for the two systems. Fe films on Co(1 0 0) surface were found to be FM up to three monolayers while it is FM only for one monolayer on Co(1 1 1) substrate. For thicker films, a sequence of AFM coupling is found for both systems with an important difference which consists in the absence of the bilayer AFM coupling in Fe/Co(1 1 1) system, whereas it is identified as the ground state for an even number of Fe monolayers on Co(1 0 0). This difference was also observed in the case of Fe films deposited on Cu(1 1 1) and Cu(1 0 0). As has been noticed by Krüger [29], we can say that this difference is probably due to the large AFM coupling between next nearest neighbours (NNN) in (1 0 0) surface, which favours the stability of this state, and it is absent in the case of (1 1 1) surface. Contrary to Fe/Co(1 0 0) where the coupling between surface and subsurface is ferromagnetic with a slight reduction of subsurface magnetic moment compared to that of the surface, this coupling is always antiferromagnetic in the case of Fe/Co(1 1 1) and leads to a strong reduction of the subsurface magnetic moment.

In the magnetic studies of fcc Fe films, it was shown that Fe/Co(1 0 0) and Fe/Cu(1 0 0) systems exhibit similar magnetic behavior [2,5]. Thus, it was concluded that, in the case of (1 0 0) surface, the ferromagnetic nature of Co substrate have a weak influence on magnetic structure of Fe films. From this result, an interesting question arises: is the magnetic structure of Fe/Co(1 1 1) similar to Fe/Cu(1 1 1)? In order to answer this question and reveal the specific properties of triangular lattice of Fe films and the polarization effect of Co on Fe magnetism, we compare systematically our results with those obtained on Fe/Cu(1 1 1) by Krüger [29]. However, it is important to notice that the magnetic structure of fcc Fe films depends sensitively on the lattice parameter. As the values of in-plane lattice constant in fcc Fe films grown on Co(1 1 1) are smaller than those of Fe/Cu(1 1 1) system, thus, it is not surprising to observe differences in the calculated magnetic structure and magnetic moments between these systems. The most important differences found are: (i) the ferromagnetic order is the ground state only for 1 ML of Fe/Co(1 1 1), while 1 and 2 MLs are ferromagnetic in Fe/Cu(1 1 1). This means that the ferromagnetism Co effect is not sufficient to align the magnetic moments in Fe films parallel. (ii) The surface and subsurface layers are always antiferromagnetically coupled in case of Fe/Co(1 1 1), whereas this coupling is systematically ferromagnetic in the Fe/Cu(1 1 1). (iii) An enhanced surface magnetic moment of Fe films is observed on both substrates, but this increase is more pronounced in Fe on Cu(1 1 1). (vi) The antiferromagnetic coupling in fcc Fe on Co(1 1 1) and Cu(1 1 1) leads to a decrease of its local magnetic moments. However, this decrease is drastic in Fe/Co(1 1 1). As it has been mentioned, this difference between the two systems may be explained by the smaller lattice parameter of Co as compared to that the Cu. In addition, we can also attribute these differences to the influence of ferromagnetic Co substrate. Indeed, the Fe–Co interaction at the interface is stronger than Fe–Cu one in the case of Fe films deposited on non-magnetic Cu(1 1 1) substrate. We can thus conclude that above one monolayer of Fe film ($n > 1$), the vanishing of ferromagnetism in Fe/Co(1 1 1) is probably due to the competition between smaller interlayer Fe distances used in Fe/Co(1 1 1) system and Co polarization effect.

Finally, the more interesting common feature between Fe/Co(1 1 1) and Fe/Cu(1 1 1) systems is the behavior of the total magnetic moment of the film (μ_{film}) with coverage n. This variation is displayed in Fig. 1b. As it has been experimentally observed in the fcc Fe films deposited on Cu(1 1 1) [24,27], the Fe films on Co(1 1 1) display also an oscillatory behavior with periodic oscillation of 2 ML. However, contrary to Fe/Cu(1 1 1) system, no transition occurs from high spin to low spin states. This is due probably to the absence of ferromagnetic order for Fe films above one monolayer ($n > 1$). The periodic nature of these oscillations, as in Fe/Cu(1 1 1) case, could be intimately related to the complex magnetic structure of bulk fcc Fe which present a spin spiral as ground state on one hand [42] and to spin density wave formation in the inner Fe on the anther hand. Indeed, in bulk fcc iron, it is well established that competition between ferromagnetic and antiferromagnetic interactions of the different nearest neighbours shells causes the frustration and leads to the spiral magnetic state [43]. As increasing film thickness effects, non-collinear effects could play an important role, than, a non-collinear calculations could provide further insight on the magnetic behaviour of this systems [43,44]. These ab initio calculations should be needed to determine in detail the ground state and the Fe film magnetic structure.

4. Conclusion

In this paper, we have presented ab initio calculations for the magnetic structure of n ($n = 1, \ldots, 6$) Fe ML films deposited on Co(1 1 1) ferromagnetic substrate. Taking into account all collinear magnetic configurations in p(1×1) unit cell, we have found that Fe film is ferromagnetic only for 1 ML. For thicker film, two almost degenerated antiferromagnetic states exist, where no ferromagnetic solutions are observed above 2 Fe ML. For all thicknesses, we have observed a strongly enhanced Fe surface magnetic moment compared to the inner layers magnetic moments.

In our study, we have compared our results with those of Fe/Co(1 0 0) system on one hand and with Fe/Cu(1 1 1) results on the other hand. We have found that the fcc Fe film on Co(1 1 1) surface is strongly different from the one deposited on Co(1 0 0) surface. However, contrary to the [1 0 0] direction where the magnetic structure of Fe/Cu(1 0 0) is similar to that of Fe/Co(1 0 0), we have found some quantitative differences in Fe/Co(1 1 1) and Fe/Cu(1 1 1) systems which are attributed to two factors: the first one is due to the smaller lattice parameter of Co used in Fe/Co(1 1 1) study compared to that of the Fe/Cu(1 1 1) system. The second, results probably from the magnetism effect of Co substrate. We have also noted the existence of an oscillatory behavior of total magnetic moment with Fe film coverage with a period of two monolayers in Fe/Co(1 1 1). This magnetic behavior is attributed to a non-collinear magnetic structure of fcc Fe bulk and a complex

geometrical (1 1 1) surfaces which favour the spin density wave formation in the inner layers of films.

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