Magnetic configurations of a Co monolayer on Cr substrates

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The spin polarization of a single Co monolayer on Cr substrates with low-Miller indices is investigated using the tight-binding linear muffin-tin orbital method. For all Cr substrates we consider epitaxial growth of Co. The Co overlayer is ferromagnetic for the (100) and (111) faces while for the (110) direction the stable solution is a $C(2\times2)$ that gives a zero net magnetization on the Co monolayer. For (100) Cr substrate the effect of the Co overlayer is to decrease dramatically the Cr polarization in the two monolayers underneath the Co and the Co-Cr coupling at the interface is found ferromagnetic. In the case of the (111) surface the effect of Co on the magnetization of the Cr substrate is less pronounced and the Co-Cr coupling is now antiferromagnetic. For the Co monolayer on the (110) surface we obtain a $C(2\times2)$ solution that gives a zero net magnetization per layer, while for the Co bilayer on Cr(110) we get a ferromagnetic configuration. In both cases the magnetic moments at the Cr interface atoms are strongly reduced.

I. INTRODUCTION

Studies of the growth process at the atomic level are of great interest for any realistic description of the magnetic map of supported transition-metal nanostructures. It is only recently that methods of sample growth, structural characterization, and magnetic measurements have been refined to the point that accurate studies have become possible. Moreover, with the increasing sophistication of our understanding of such phenomena as interface anisotropy, giant magnetoresistance, and interlayer coupling, the role of the interface magnetic moments is becoming recognized as increasingly important. New impetus in this field has been recently given by the application of scanning tunneling microscopy (STM) studies to the structural characterization of ultrathin magnetic films. In addition new magnetic microscopy techniques have emerged, notably magnetic force microscopy, spin-sensitive STM, near optical magneto-optical Kerr effect (MOKE), the application of advanced lithography, and pattern transfer techniques to the fabrication of nanoscale magnetic elements based on ultrathin magnetic films.[1]

Among artificially layered metallic systems, those containing magnetic/nonmagnetic and ferromagnetic/antiferromagnetic interfaces have received the highest attention. Probably the Fe/Cr interface systems have been the most extensively studied not only for the fundamental interest but also for the technological applications.[2,3] The Co/Cr interface systems exhibit, in principle, similar favorable conditions but they have been not so widely analyzed, probably due to the difficulty of producing Co/Cr samples of good quality (Fe and Cr have in bulk the same bcc structure and nearly the same lattice constant while Co and Cr exhibit different stacking and lattice constant in their respective stable bulk configuration). For those reasons the case of Co films deposited on Cr substrate has only begun to be examined.

In the early 1990s Scheurer *et al.*[4,5] pointed out that Co grows in a metastable bcc or tetragonal phase on Cr(100) at room temperature. These authors have shown, using low-energy electron diffraction (LEED) analysis, that cobalt layers grown at room temperature on Cr(100) nearly reproduce the structure of the substrate, thus leading to a metastable cobalt bcc phase. This result has been confirmed by different authors.[6–8] These authors have shown that in Co/Cr(100) superlattices, the first monolayer (ML) of Co grows with a pseudomorphic bcc structure. With increasing Co thickness the structure relaxes back continuously into the intrinsic hcp structure with the *c* axis in the plane parallel to Cr(110).[6,7]

Very recently, Fölsch *et al.*[9] succeeded in preparing pseudomorphic Co growth on a Cr(110) substrate. Later on they reported[10] investigations by magnetic dichroism in photoemission in conjunction with complementary magneto-optical Kerr effect (MOKE) measurements. From both experiments they concluded that the Co films (9 ML in the dichroism measurements and 6.5 ML in the MOKE measurements) display ferromagnetic order.

These Co/Cr interface systems have not been widely studied theoretically even if perfect abrupt interfaces are considered (perfectly layered materials). The difficulty of treating this interface from the theoretical point of view arises mostly from the complex behavior of Cr. Theoretical calculations mimic the Cr substrate by considering a slab of *n*-Cr layers as thick as to assure that the magnetic behavior at the interface does not depend on the slab thickness. For other metals the surface can be simulated by considering only a few layers, while for Cr a huge number of monolayers have to be considered (more than 20), increasing strongly the computational time needed. Also most of the codes work essentially in the local-density approximation (LDA) which is not really suitable to describe, in a satisfactory way, transition-metal elements like Cr or Mn. It is therefore desirable to go ''beyond LDA''[11] in order to get a satisfactory description of the magnetic properties of a Cr interface. Moreover Cr exhibits an incomensurate spin-density wave (SDW) in bcc bulk[12] that has been treated rarely in theoretical studies, and the

presence of a similar SDW in Cr substrate systems is expected. So far there exist only a few semiempirical and simplified *ab initio* calculations for Cr clean surfaces, while for Co/Cr interfaces only very few studies concerning ultrathin Co/Cr multilayers are available.

In order to analyze the dependence of the magnetic behavior of the Co monolayer (ML) on Cr substrates with crystallographic orientation, we have performed *ab initio* tight-binding linear muffin-tin orbital (TB-LMTO) calculations for three different faces (100), (110), and (111). To perform these calculations we have replaced the semi-infinite substrate by a three-dimensional lattice in which a supercell consisting of metallic slabs separated by empty space is used. This TB-LMTO code has already produced valuable results in the case of Fe/V superlattices and for thin V films on Fe(001) and Fe(110).[13] Also, Robles *et al.*[14] have determined the magnetic polarization of a Co monolayer on Pd(110).

The paper is organized as follows. In Sec. II we briefly comment on the theoretical model. In Sec. III A, we present the results obtained for the Cr substrate, and then in Secs. III B–III D we report on the magnetic map of, respectively, Co/Cr(100), Co/Cr(110), and Co/Cr(111). The main conclusions of the present study are summarized in Sec. IV.

II. THEORETICAL MODEL

The calculations are performed using a scalar-relativistic version of the *k*-space TB-LMTO method[15,16] with the atomic-sphere approximation. This method is usually based on the local-spin-density approximation[17] of the density-functional theory.[18] Within this approach we have first determined the lattice parameter of Cr bcc bulk by minimization of the total energy. The magnetic moment obtained is not in good agreement with experimental results so that, as discussed by Moroni and Jarlborg,[19] it is necessary to go beyond the local-spin-density approximation (LDA) to generalized-gradient-approximation (GGA). The Langreth-Mehl-Hu[20] and Perdew-Wang[21] GGA functionals have been tested in the present communication and the Langreth-Mehl-Hu was retained because it gave the best agreement with experimental results.

The Cr substrate has been replaced by a *n*-layer-film of Cr. We have taken for *n* a value big enough to reproduce, at the center of the slab, a magnetic moment very similar to that of Cr bulk. On each side of the Cr slab we have added Co ML assuming bcc pseudomorphic epitaxial growth, i.e., the Co atoms are placed in the continuation of the Cr substrate atoms following the bcc structure.

The calculations are performed using an increasing number of *k* points, until final convergence is obtained for about 150 *k* points in the irreducible Brillouin zone. We have also considered enough layers of empty spheres to assure that there is no interaction between the Co surfaces of adjacent supercells[22] (five monolayers of empty spheres).

We have considered nonmagnetic and different types of magnetic configurations. For the (100) and (110) orientations both the the in-plane antiferromagnetic $C(2\times2)$ configuration and the ferromagnetic (FM) configuration have been studied. In order to get reliable energy difference between FM and $C(2\times2)$ configurations we have done all our numerical calculations for the (100) and (110) surfaces with two inequivalent atoms per plane. Thus the energies determined are for the same number of atoms in the unit cell, the same irreducible Brillouin zone; also the same number of *k* points have been used. In the case of the (111) substrate, besides the usual FM configuration we have also considered several different ''nonferromagnetic'' configurations discussed by Krüger *et al.*[23] in the case of $3d$ elements on graphite [same hexagonal surface as (111)]. More recently Krüger *et al.*[24] have also reported on those ''nonferromagnetic'' configurations for $3d$-transition-metals atoms on Cu(111) and Ag(111). Therefore, for this (111) orientation and for the nonferromagnetic configurations, we had to take into account in general more than two inequivalent atoms per plane.

III. RESULTS AND DISCUSSION

A. Cr surface

Cr bulk is known to be bcc with an experimental lattice distance of 5.44 a.u. and shows antiferromagnetic ordering (AF) with a magnetic moment per atom of about $0.60\mu_B$.[25–27] Moreover, as discussed in detail by Fawcett,[12] chromium metal exhibits a great number of complex magnetic phenomena, and a well-known incommensurate spin-density wave (SDW). The electronic structure calculations for the incommensurate SDW state itself has seldomly been carried out[28,29] due to the computational difficulties (at least 40 inequivalent Cr atoms for the minimum bcc bulk shell have to be considered), and usual *ab initio* calculations for Cr bulk[30,31] have been confined to the commensurate SDW antiferromagnetic state (AF). Our goal in this work is not to study extensively the Cr bulk but to examine the effect of crystallographic orientation on Cr surface and Co/Cr interfaces. The presence of the incommensurate SDW in Cr(110) surface has been found experimentally by Schäfer *et al.*,[32] but Niklasson *et al.*[33] calculated that for perfect Fe/Cr interfaces no nodes of the SDW in the Cr film should appear near the interface layers. From this work it can be infered that the polarization at the Cr surface and the Co/Cr interface should not vary substantially if only the commensurate AF Cr SDW is considered in the calculations.

The first step to study the Cr surface should be to reproduce the structure and magnetic properties of the Cr bulk within our model. We use in our *ab initio* TB-LMTO study the GGA aproximation of Langreth-Mehl-Hu[20] (see theoretical model) choosing enough number of *k* points to assure convergence in energy and stability in the magnetic moments. The AF arrangement for bcc Cr bulk is obtained as the stable configuration with a magnetic moment of $0.63\mu_B$ per atom and a lattice distance of 5.41 a.u. for the energy minimum. The Cr-Cr distance will be fixed to this value for all the following calculations.

We simulate the Cr surface by taking a slab of *n* Cr layers thick enough such that the magnetic properties of the surface do not vary substantially with the slab size and also to get at the central Cr layer a similar behavior as in the Cr bulk. Cr is a very sensitive element and a large number of Cr layers are needed to mimic the bulk in the center. In Fig. 1 we display the magnetic moments in a 29-ML Cr slab in the (100) orientation. Only after more than ten Cr underlayers do we aproach bulk conditions. Working with such a large amount

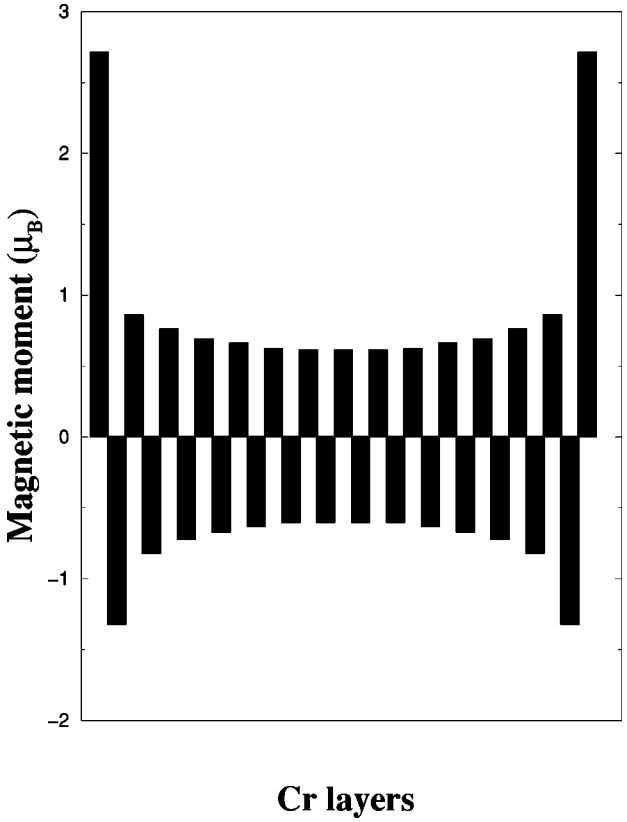

FIG. 1. Magnetic profile (in μ_B) of a 29-layer slab of Cr in the (100) orientation simulating the Cr(100) surface. The Cr bulk magnetization ($0.63\mu_B$ in our calculation) is only reached after ten underlayers. Typical AF Cr arrangement is also present in the sample.

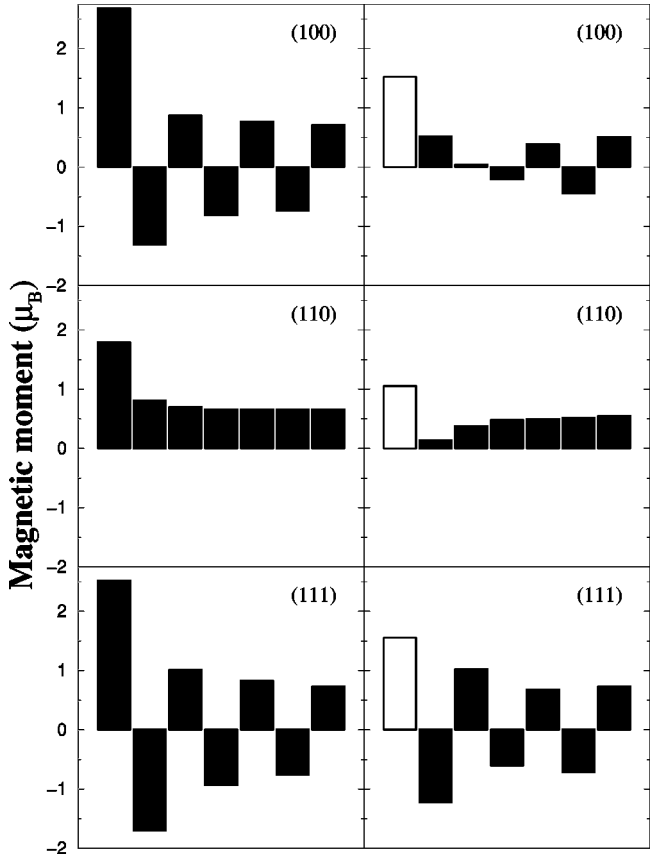

FIG. 2. Local magnetic moments at the inequivalent atoms of the Cr surface (left side) and a Co monolayer on Cr (right side) for (100), (110), and (111) orientations (upper, middle, and bottom panels, respectively) where open bars correspond to Co interface and black bars correspond to the Cr slab layers. For (100) and (111) systems we find a FM configuration as the stable solution of our calculations, while for (110) we obtain a C(2×2) configuration (two inequivalent sites per layer) for the minimum in energy. For this C(2×2) configuration we display the absolute values of the magnetic moments at the different sites.

of layers to simulate Cr surface increase strongly the computing time of the calculations.

For all the geometrical orientations [(100), (110), and (111)] we have considered nonmagnetic and several magnetic configurations at the surface of Cr, but, in principle, only a few of them seem to be probable, i.e., those displaying the typical AF structure of Cr bulk at the interior.

In Fig. 2 (left side) we show the magnetic moments at Cr inequivalent sites for (100), (110), and (111) Cr surface, going from the Cr surface to inner layers of the slab.

Cr(100): The first experimental evidence for FM ordering in the Cr(100) surface was provided by Rau and Eichner[34] using electron-capture technique. Afterwards angle-resolved photoelectron spectrocopy measurements of Klebanoff *et al.*[35,36] showed the same FM ordering at the surface with magnetic moments of $2.4\pm0.3\mu_B$ per atom as well as the AF coupling between Cr(100) surface and the first Cr underlayer. In our calculation the stable magnetic solution for this system is a layer-by-layer AF configuration for the system (namely layered AF), which is the only one that leads to the bulk AF arrangement in the interior of the slab of Cr. The atoms at the surface display high magnetic moments ($2.68\mu_B$, more than four times Cr bulk magnetization), and the value of the magnetic moment is reduced in going from the surface to inner layers of Cr to approach the bulk limit after the fifth underlayer. Our results are in qualitative agreement with earlier semiempirical studies[37–41] for thin films of Cr in this orientation, and in good agreement with the TB-LMTO result ($2.61\mu_B$) of Alden *et al.*[42] However, in this work,[42] the authors mimic the Cr(100) surface using thinner slabs of Cr (6 ML) and consider the LDA approximation that leads, in their work, to magnetic moments of about $0.40\mu_B$ for the central layer and $0.21\mu_B$ for the Cr bulk in their calculations (far away from the experimental $0.60\mu_B$ for Cr bulk). Our results are also in agreement with the experimental data cited above.

Cr(110): In this case, the only simple solution that leads to AF ordering at the center of the slab is a surface C(2×2) configuration, and is also the most stable in our calculations. In this configuration there are two inequivalent Cr atoms per layer, and each atom of one type is surrounded by four atoms of the other type. The magnetic moments of the two inequivalent sites are aligned antiparallel so that the net magnetization per layer is zero. The local magnetic moments per atom at the surface are high ($1.80\mu_B$) but less that in the (100) surface, and decrease quickly to recover the Cr bulk magnetization after a few Cr underlayers. These data are in qualitative agreement with semiempirical calculations of Victora *et al.*[40] and the TB-LMTO result ($1.39\mu_B$) of Alden *et al.*[42] (for a 6-ML slab of Cr and using LDA instead of GGA, as commented in the previous paragraph). The number

of layers needed to reach de Cr bulk behavior is less than in the previous (100) surface, mainly due to the different interlayer distance which in the (110) orientation is $\sqrt{2}$ times the interlayer distance in the (100) orientation.

Cr(111): Also for this surface the layered-AF solution produces AF ordering in the interior of the slab and is energetically the most stable. The magnetic moments displayed at the surface atoms are very large ($2.52\mu_B$) and comparable in value to the (100) orientation. Moreover, the decrease of the magnetic moments as going from surface to inner layers is slightly slower than for the (100) case. The interlayer distance in this orientation is $\sqrt{3}/3$ the distance in (100) orientation.

B. Co ML on Cr(100) substrate

Scheurer *et al.*,[4,5] pointed out that Co grows in a metastable bcc or tetragonal phase on Cr(100) at room temperature. More recently other groups[6,7] have studied and characterized the growth proccess of Co on Cr(100) in Co/Cr(100) superlattices. Using molecular-beam-epitaxy technique (MBE) they have produced superlattices of different thickness (5–50 Å), studying their structure by diffraction techniques. For Co depositions equivalent to 2 or more monolayers the diffraction patterns show that Co grows following its usual hcp stacking, while for a single overlayer of Co on Cr(100) they conclude that the growth is pseudomorphic and in bcc phase. The forced bcc stacking at very low coverages of Co is due to Cr(100) surface potential and to the good fitting of the Co(110) plane on Cr(100), that gives a reasonable stability of this growth orientation for the first monolayer of Co on Cr(100). The competition between the Cr(100) surface potential and the bulk potential of hcp Co leads to a bcc-hcp face transition for thicker coverages.

Following the experimental data we assume in our calculations pseudomorphic bcc growth of a single Co monolayer on Cr(100). The Cr surface is simulated with a *n*-ML slab of Cr in the (100) orientation. The central layer of the slab would be the equivalent of the Cr bulk in the sample. Also in the neighborhood of the central layer Cr should exhibit its characteristic AF bulk magnetic arrangement. This behavior is difficult to obtain taking a few Cr layers in the slab so, at least in this case, a slab of 17 layers is needed to get reasonable stability of our results. The Co atoms in the overlayer are placed pseudomorphically on Cr, following the bcc stacking with the Co-Cr distance equal to the Cr bulk lattice parameter. Nonmagnetic and several magnetic configurations of the system have been considered in our calculations, but due to symmetry and the AF arrangement of the Cr bulk, only pure FM and layered-AF ones seemed to be reasonable for this orientation. Nevertheless, in order to be be complete, we have also considered the C(2×2) configuration as input in the self-consistent loop: this configuration is unstable and leads to the solution reported in Fig. 2.

In Fig. 2 (right side, upper panel) we display the magnetic moments for the inequivalent sites of Co and Cr in Co/Cr(100) sample for the minimum energy configuration. The Co overlayer is magnetic with a valuable magnetic moment of $1.46\mu_B$. This magnetic configuration is found to be 11 mRy per Co atom more stable than the nonmagnetic solution. For the sake of comparison we have also calculated

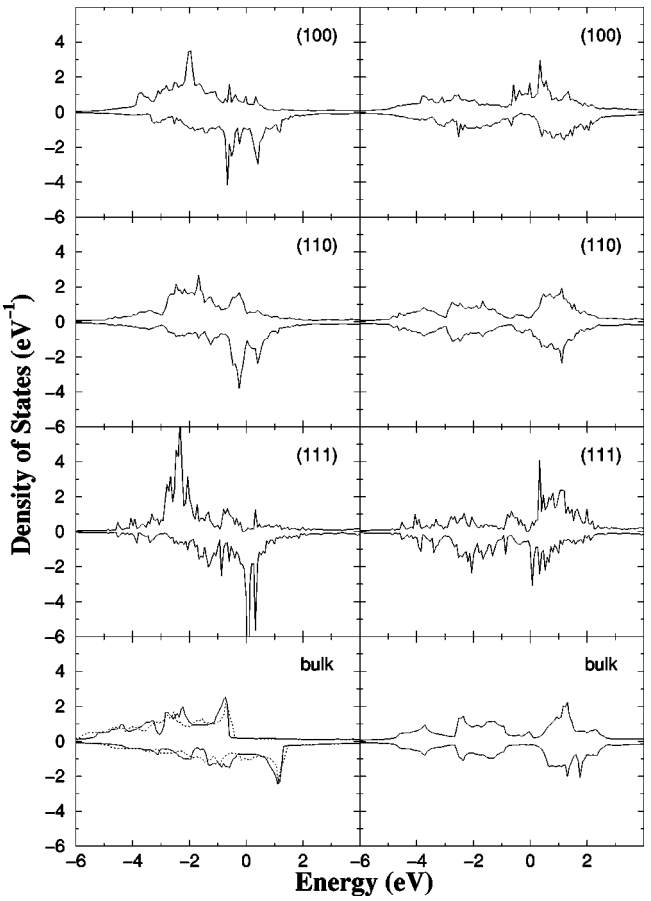

FIG. 3. Total density of states for Co atoms (left panel) for different systems: Co monolayer on Cr for (100), (110), and (111) orientations (first, second, and third graphs) and Co hcp and fcc bulk (bottom graph, solid line, and dashed line, respectively). The total density of states for the Cr interface atoms in these systems and Cr bulk is plotted in the right panel. The Co-Cr interaction at the interface is reflected in the structure at the density of states above the Fermi level of Co interface atoms which is not present in Co bulk.

using the TB-LMTO method the magnetic moment of a free standing monolayer of Co cut in the (100) orientation of bcc stacking and with the same distances as in bulk Cr. The magnetic moment of Co atoms in this system is $2.15\mu_B$, so the magnetization of Co atoms decrease, not only from the increase of the coordination number but also from the Co-Cr interaction. The hybridization of the Co atoms with the Cr substrate is reflected in the density of states shown in Fig. 3. Comparing the Co surface atoms with bulk Co, even if Co bulk is not bcc, the presence of some structure in the density of states of Co surface atoms above the Fermi level corresponds to the interaction with the Cr substrate which has a strong structure in that area.

The Cr atoms at the interface have a net magnetization of $0.45\mu_B$, and are ferromagnetically coupled with the Co surface. Herman *et al.*[43] have found the same ferromagnetic coupling between Co and Cr at the interface of ultrathin Co/Cr(100) superlattices. As going to the second underlayer the magnetization of Cr atoms is strongly reduced due to the competing effect of Co-induced ferromagnetic polarization and the AF arrangement of Cr in the Cr(100) slab (see the Cr

TABLE I. Local magnetic moments (μ_B) at the inequivalent atoms (two per layer in the double cell) of a single Co monolayer and a Co bilayer on Cr(110) for the stable configuration in our calculation. Co_S and Co_I correspond to surface and interface of Co, while Cr_I and Cr_{I-n} are Cr atoms at the interface and the following underlayers. For the Co monolayer we obtain a C(2×2) solution that gives a zero net magnetization per layer, while for the Co bilayer on Cr(110) we get a FM configuration.

	Co_S	Co_I	Cr_I	Cr_{I-1}	Cr_{I-2}	Cr_{I-3}	Cr_{I-4}
Co/Cr(110)		1.05/−1.05	−0.13/0.13	0.38/−0.38	−0.48/0.48	0.50/−0.50	0.52/0.52
Co_2/Cr(110)	1.83/1.83	1.60/1.60	0.13/0.11	−0.04/−0.03	0.01/0.00	−0.01/0.00	0.02/−0.01

surface for this orientation). The effect of the Co overlayer is extended until a few monolayers in the Cr substrate.

In the experimental studies[6,7] the authors noted an expansion of the Co-Cr interlayer distance of about 6% as compared with the usual Cr bulk lattice. In order to verify the effects of relaxation in our study for this orientation we have considered an expansion of this magnitude in the interface Co-Cr distance in our samples. The trends obtained are the same and the value of the magnetic moments differs by a factor similar to the relaxation, so that we can conclude that the possible mismatch in the interface Co-Cr distance is not crucial for the magnetic arrangement of the system.

C. Co ML on Cr(110) substrate

Very recently Fölsch *et al.*[9,10] have published two experimental papers concerning Co films on Cr(110) substrate. In the first,[9] using MBE techniques, they deposited different coverages of Co (from 1 ML to 30 ML thicknesses) on the Cr(110) surface and then they examined the structural details by high-resolution low-energy electron diffraction (LEED) technique. In the second,[10] they present a study of the electronic and magnetic properties of these samples by magnetic dichroism and MOKE. They observed that Co grows pseudomorphically on Cr(110) from very low depositions (first Co overlayer) until relatively thick coverages (30 ML), following the bcc stacking of Cr for a deposition of at least ten Co ML. They find no significative mismatch between Co-Cr and Cr-Cr distances at the interface. Diffraction patterns show a significant two-domain (3×1) reconstruction due to the lattice distortion along in-plane atom row directions of Co on Cr. Moreover, the magnetic dichroism measurements suggest an in-plane magnetization of the Co film.

As in the previous case we mimic the system by taking a slab of *n* Cr layers simulating the (110) Cr surface and then putting the Co overlayer pseudomorphically on the Cr surface. In our calculations we have considered various magnetic configurations obtaining the C(2×2) solution as the ground state (4 mRy per Co atom more stable than the nonmagnetic configuration). Simple ferromagnetic configurations were not found as stable solutions for this sample in our calculations. When considering the ferromagnetic configuration as the input in our model, during the calculation procedure it turned to converge towards the C(2×2) solution. This C(2×2) configuration leads to an AF ordering in the center of the Cr slab as reported in the real system (Cr bulk is AF). In Fig. 2 (right side, middle panel) we present the absolute value of the local magnetic moments at the inequivalent sites of Co and Cr in the sample. Although the net magnetization of the Co layer for this configuration is zero, the local magnetic moment at each Co atom is $1.05\mu_B$. The magnetic moments at the Cr interface atoms are $0.13\mu_B$, and the magnetization recovers nearly Cr bulk value after a few underlayers.

Experimental results[10] seem to indicate that there exists an in-plane magnetization on the Co film in a Co_9Cr(110) sample while our theoretical C(2×2) configuration for a Co monolayer on Cr(110) [Co1Cr(110)] leads to a nonmagnetic Co surface. To clarify this point we have studied the magnetic properties of a Co bilayer on Cr(110) [Co2Cr(110)], assuming the same pseudomorphic growth as in the previous case. In Table I we display the local magnetic moments in all the inequivalent sites of the system (two in each layer), comparing them with the results obtained for a single Co overlayer on Cr(110). We observe that C(2×2) is no longer the stable solution of the system due to the strong ferromagnetism of Co, finding a FM configuration as its ground state. Co atoms at the surface exhibit a strong magnetization ($1.83\mu_B$), while in the second Co layer the magnetic moments are slightly reduced ($1.60\mu_B$) due to higher coordination and to the Co-Cr interaction at the interface. Cr couples ferromagnetically with the Co atoms at the interface with small magnetization ($0.12\mu_B$), and several ''dead magnetic Cr layers'' appear as going to the center of the Cr slab, beginning to recover the AF arrangement of the Cr bulk only after more than ten underlayers. So, from our calculations we infer that for thicknesses of the Co film of more than two monolayers the Co slab may exhibit a ferromagnetic character with valuable magnetic moments at the surface, in agreement with the measurements of Fölsch *et al.*,[10] while for a Co ML on Cr(110) we obtain only a C(2×2) ordering at the Co surface.

D. Co ML on Cr(111) substrate

There is no available experimental data of this system either from the structural or electronic point of view. The bcc pseudomorphic growth of a single overlayer of Co on Cr(111) seems possible. There is a mismatch of about 10% between Cr-Cr in-plane distance at the Cr(111) surface and the closest Co-Co distance in hcp Co bulk. So the forced bcc stacking would come from the competition between the surface potential of Cr(111) and the stress due to the lattice missmatch between Cr-Cr in the sample and Co-Co in hcp bulk, while for thicker coverages, the stress would lead to a reconstruction.

For our calculation we consider, as in the other cases, pseudomorphic growth of a single Co ML on Cr(111). The modeling of the theoretical system is similar to the other cases, and we have considered nonmagnetic and various

magnetic configurations (not only the simple FM ones but also several more complex solutions proposed by Krüger *et al.*[23,24]) but only the FM configuration survives after a few self-consistent loops.

The magnetic moments for each inequivalent Co and Cr atoms in the sample are shown in Fig. 2 (right side, bottom panel). The Co surface has a valuable magnetization of $1.55\mu_B$ (the magnetization of a free standing Co monolayer calculated with our method for this orientation is $2.25\mu_B$), while the Cr interface couples now antiferromagnetically with Co atoms with magnetic moments of $1.20\mu_B$. This magnetic configuration is found to be 26 mRy per Co atom more stable than the nonmagnetic one. The hybridization between Co surface atoms and the Cr interface is reflected in the presence of some strong structure above the Fermi level in the density of states (Fig. 3). In going deeper in the Cr slab the magnetization reduces obtaining nearly the Cr bulk value after a few Cr layers.

The antiferromagnetic coupling at the Co/Cr interface for this orientation is a surprising, feature. To assure that this result is not an artifact due to the small thickness of the Cr slab, we have studied different samples considering different thicknesses of the Cr slab, and in all the cases we have obtained this behavior for up to 30 layers in the Cr slab. Another fact is the possible dependence of the results on the Co-Cr distance at the interface, but we have calculated these systems considering a small (from 5% to 15%) reduction or expansion of the interface distance and the antiferromagnetic coupling was still present. This behavior could be due to the different coordination for Co and Cr at the interface for the different orientations. In the (111) direction the average coordination number for the Cr interface atoms is reduced as compared with (100) orientation. This means that the mean number of Co neighbors of each Cr atom is less in the (111) orientation than in the (100). This could be the reason for the different behavior for these two different systems.

IV. SUMMARY

In this paper we have reported the magnetic map of a Co monolayer on Cr substrates. For the (100) and (110) orientations the Co overlayer reduces dramatically the polarization of the Cr substrates not only at the Co-Cr interfaces but also more deeper inside the substrate, while for (111) orientation Cr atoms at the interface have a valuable magnetization. For the (100) Cr substrate we have obtained a ferromagnetic coupling at the Co-Cr interface. This is in agreement with previous calculations by Herman *et al.*[43] displaying ferromagnetic coupling at the Co-Cr(100) interfaces in Co/Cr superlattices. In the case of a Co monolayer grown epitaxially on a Cr(111) substrate the Co-Cr coupling is antiferromagnetic. For one Co ML on Cr(110) a C(2×2) arrangement for the Co surface is obtained, while for the Co bilayer on Cr(110) the Co surface display FM ordering. Our results for the Co bilayer are in agreement with the experimental measurements of Fölsch *et al.*[10] for thin films of Co on Cr(110). Unfortunately no structural experimental data is available for the first steps of growth of Co ML on Cr(110).

We hope that the present results will give some new impetus to the experimentalist because—to date—the experimental results on these systems are very scarce.

ACKNOWLEDGMENTS

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