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Interface-driven manipulation of the magnetic anisotropy of ultrathin Co films on Pt(111): Substrate deposition of hydrogen and model calculations

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The magnetic anisotropy energy (MAE) and the resulting spin-reorientation transitions of Co/Pt(111) ultrathin films are investigated by manipulating the Co/Pt interface with controlled adsorption of hydrogen prior to Co deposition. *In situ* low-energy electron-diffraction and surface magneto-optical Kerr-effect measurements are performed on Co films grown at low temperatures. The results show that interface H deposition leads to a remarkable change in the magnetization direction from perpendicular to in-plane, even for the thinnest Co films, which is accompanied by an important increase in the coercive force. Layer-resolved self-consistent electronic calculations of the MAE are performed in order to identify the interface contributions responsible for perpendicular magnetic anisotropy (PMA) and to quantify how the MAE depends on various possible adsorbate-induced modifications in the local magnetic moments. The results show that the PMA is quite insensitive to changes in the local magnetic moments at the Co film surface even if they are relatively large. However, the PMA depends crucially on the Co-interface moments, on the Pt-interface moments induced by the proximity to Co, and on the resulting spin-orbit interactions at the Pt atoms. The observed suppression of PMA by interface H adsorption is interpreted as the consequence of the reduction in the interface-Pt moments which, originates either a reduction in the Co-interface moments or at a decoupling of the Pt substrate from the magnetic film. Experiment and theory thus prove the dominant role of the Co-Pt interface MAE on the development of the relative stability of perpendicular and in-plane magnetization directions. The magnetic properties of ultrathin films may thus be tailored to a large extent by adsorbates trapped at 3*d*-4*d* or 3*d*-5*d* film-substrate interfaces.

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I. INTRODUCTION

In past years thin films and layered magnetic materials have been the subject of an intense research activity, which is driven by both the fundamental interest of low-dimensional magnetism and the numerous perspectives of applications in spintronics and memory devices.[1–5] Ultrathin films involving 3*d*-4*d* and 3*d*-5*d* interfaces such as Co/Pd, Co/Pt, Co/Au, and some related alloys have attracted particular attention in this context since they often show an easy magnetization axis that is perpendicular to the film, a phenomenon known as perpendicular magnetic anisotropy (PMA).[6–8] These new materials fulfill the requirements for perpendicular magneto-optical recording media and are therefore expected to play an important role in high-density storage technology. A detailed understanding of the microscopic origin of PMA is crucial for the development of new methods for tailoring the magnetoanisotropic behavior of thin films and nanostructures.

The PMA and, in particular, the stability of the off-plane easy axis, have been initially interpreted to be the result of the magnetocrystalline contributions of the 3*d*-4*d* or 3*d*-5*d* interfaces, which overcome the classical magnetostatic dipolar energy. Layer-resolved electronic calculations have provided a rigorous microscopic basis for this interpretation.[9–12] Moreover, theory has revealed the internal magnetic structure of the relevant interfaces and the dominant role played by the 4*d* or 5*d* support, on which magnetic moments are locally induced.[12] Since the dipolar contributions increase approximately linearly with film thickness and always favor an in-plane magnetization, it is clear that the perpendicular easy axis is a specific ultrathin-film effect. In fact, beyond a critical thickness t_c, a so-called spin-reorientation transition (SRT) occurs, in which the easy axis shifts from off-plane to in-plane.[13–15] Moreover, this SRT often involves an intermediate spin-canted phase.[12,16] Finally, for film thickness $t > t_c$ the magnetization remains parallel to the film, showing a more or less important in-plane anisotropy, depending on its symmetry.[17–19]

Surface adatoms, surfactants and overlayers may be used to tailor the structure, morphology, and electronic properties of ultrathin films by modifying the film-vacuum interface or simply by replacing it by a different one (e.g., in the case of overlayers). In addition, adsorbates may react chemically with the film, thereby altering profoundly its electronic and magnetic properties. For instance, oxygen exposure of the highly reactive magnetic transition metal atoms is known to cause the formation of antiferromagnetic oxide layers or even to quench magnetism completely. In the later case the nonmagnetic interface material, are usually referred to as magnetic dead layers.[20] The presence of inhomogeneities associated to surfactants may also affect the dynamics of magnetic domain walls (DW) by changing the nucleation field for DW formation and by introducing new pinning centers which condition the DW propagation. In this way the coercive field and the magnetization reversal process can be tuned. Moreover, surfactants can be useful in order to manipulate the surface roughness and the growth mode. For example, surfactants could induce changes from hcp to fcc phases. They can also suppress the formation of twin boundaries, in a similar way as low-temperature growth does.[21,22] Such changes of symmetry and local environment are clearly expected to affect significantly the magnetoanisotropic film properties.

Recently, several investigations have been reported on the role of adsorbed gases (e.g., CO, O_2, H_2, etc.) on the magnetic properties of ultrathin films, particularly concerning PMA. In most cases the gases are adsorbed on the film surface (i.e., film-vacuum interface), for example, CO on $Co_m/Pt(111)$, H, CO, and O on $Co_m/Pd(111)$, and H and CO on $Ni_m/Cu(001)$.[20,23–25] These post-growth adsorption experiments have the advantage of allowing a simple and direct comparison of the effects of the adsorption on the magnetic behavior. Moreover, they address and manipulate the surface of the film, which is of course crucial for conferring the low-dimensional character on the magnetic material. However, the surface is not the only magnetically relevant interface in the system. In fact, when global film properties are concerned, such as the magnetic anisotropy energy (MAE) and the orientation of the easy axis, the film-substrate interface is equally important *a priori*. In fact, in the case of the PMA of Co films on highly polarizable substrates (e.g., Pd or Pt) it is the film-substrate interface, rather than the film-vacuum interface, what dominates the subtle magnetoanisotropic phenomena. Moreover, in the ultrathin limit the interaction or interference between the interfaces is not negligible. It is therefore, of considerable interest to investigate the role of film-substrate interface.

An alternative approach, which focuses on the film-substrate interface, consists in adsorbing the gas on the substrate surface *before* the magnetic film is grown. This perspective has been adopted in recent studies involving O_2, namely, Ni/O/Cu(001), Fe/O/Fe(001), and Ni/O/Cu(110) as well as Co, Fe, and Ni on O/Cu(001).[26–28] In the present work we have considered H as a specific adsorbate for manipulating the magnetic properties. Hydrogen is a common adsorbate in a variety of surface-science studies and appears to be a good candidate for the modification in epitaxial growth on both metal and semiconductor surfaces. It undergoes dissociative adsorption on a Pt(111) surface which involves the H 1*s* and Pt 5*d* orbitals. At room temperature the dissociated H ions seem to be delocalized or disordered while at low T they form an ordered 1×1 overlayer for saturation coverages.[29] Experiments show that H chemisorbs preferentially at threefold hollow sites, which is also in agreement with calculations at high coverage. However, at low coverages it does not show a strong preference among the different high-symmetry adsorption positions (top, bridge, hcp or fcc) and may even display quantum tunneling effects due to its small mass.[29,30] Interestingly, H deposition on surfaces has been used to reduce interfacial mixing in the growth of multilayered films since it inhibits the exchange-atom diffusion mechanism in favor of the hopping.[31] In the specific case of Co/Pt interfaces, interdiffusion and interface alloying become important only at temperatures well above room temperature.[32–35] Finally, it is also interesting to mention that photoemission studies have shown that H chemisorption causes strong reduction in the Fermi-level density of states at the Pt surface atoms,[36] which should directly affect the magnetic susceptibility of the substrate.[37,38] Therefore, one expects that by adsorbing H_2 on the Pt(111) surface prior to the deposition of the Co film should allow us to manipulate directly the film-substrate magnetism, in particular, the magnitude of the Co and Pt interface moments and consequently the PMA.

The remainder of the paper is organized as follows. In Sec. II the experimental results on $Co_m/Pt(111)$ are reported. Results are given for both Co films on clean Pt(111), as well as for the most interesting Co films grown on a Pt(111) substrate, that was previously exposed to H_2. The corresponding discussion of the experimental findings motivates the theoretical investigations presented in Sec. III. Layer-resolved self-consistent calculations of the MAE are presented together with an analysis of the microscopic origin of the magnetoanisotropic properties from a local perspective. The effect of adsorbates on the different atomic layers is simulated by varying the strength of the local magnetic moments at the film surface, at the Co atoms in contact with the Pt substrate, and at the interface Pt atoms. A summary of conclusions is given in Sec. IV.

II. EXPERIMENTAL RESULTS

A clean Pt(111) surface was obtained after several cycles of Ar^+ sputtering and short annealing treatments to 900–1000 °C. Oxygen treatments consisting in exposures at 2×10^{-7} mbar for a few minutes at a temperature of 700 °C were also performed in order to remove residual surface carbon contamination. In all measurements the same Pt single crystal was used without changing the crystallographic orientation of the magnetic field. In fact, the Pt substrate was never taken out of the chamber throughout the whole series of reported experiments. The orientation of the in-plane crystallographic axes is deduced from the low-energy electron diffraction (LEED) images. The in-plane magnetic field was applied close (within some $5°-10°$ of misalignment) to one of the directions connecting nearest-neighbor atoms (e.g., the $[1\bar{1}0]$ direction). Since the (111) surface has an hexagonal symmetry, there is a pretty weak in-plane anisotropy. Therefore, the magnetic behavior should be rather insensitive to the orientation of the applied magnetic field within the surface plane.

The exposure of the clean Pt surface to the H_2 gas was controlled by a leak valve, using a residual gas analyzer to track partial gas pressures. The background pressure in the ultrahigh vacuum chamber was in the low 10^{-10} mbar range. The Co films were e-beam evaporated with rates of about 0.10–0.20 monolayer/min. The thickness and rates were monitored by using the evaporation flux, which was previously calibrated by a quartz micro balance and x-ray photoelectron-spectroscopy measurements. Magnetic hysteresis loops were measured *in situ* via polar and longitudinal magneto-optical Kerr effect (MOKE) with a maximum applied field of 1150 Oe out-of-plane and 700 Oe for the out-

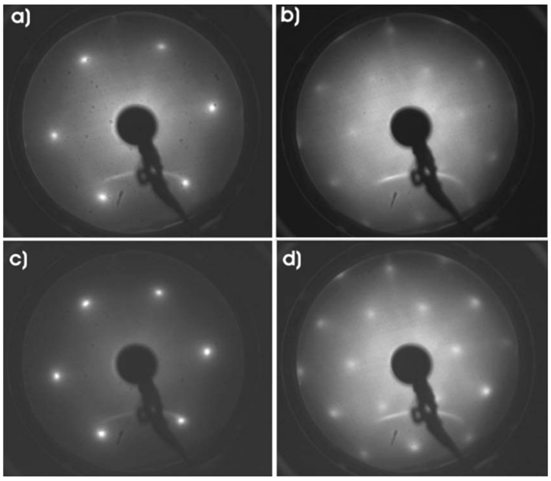

FIG. 1. LEED patterns of unexposed 24.6 Å thick Co films grown on Pt(111) at [(a) and (b)] 300 K and [(c) and (d)] 200 K. The primary electron beam energies are [(a) and (c)] 122.5 eV and [(b) and (d)] 252 eV.

off-plane and the in-plane direction, respectively. The MOKE setup uses modulation of the incoming laser polarization by a photoelastic modulator.[39]

A. Unexposed films

Many previous MOKE studies of Co on Pt grown at room temperature show that a SRT from perpendicular to in-plane easy axis occurs at around 1 nm thickness.[13] However, much fewer works have been done regarding the growth at low temperatures. In fact, films deposited at 200 K are closer to the ideal layer-by-layer growth than the room-temperature ones. This can be recognized at the higher contrast (sharper spots and a lower diffuse background) of the LEED patterns shown in Fig. 1.[22]

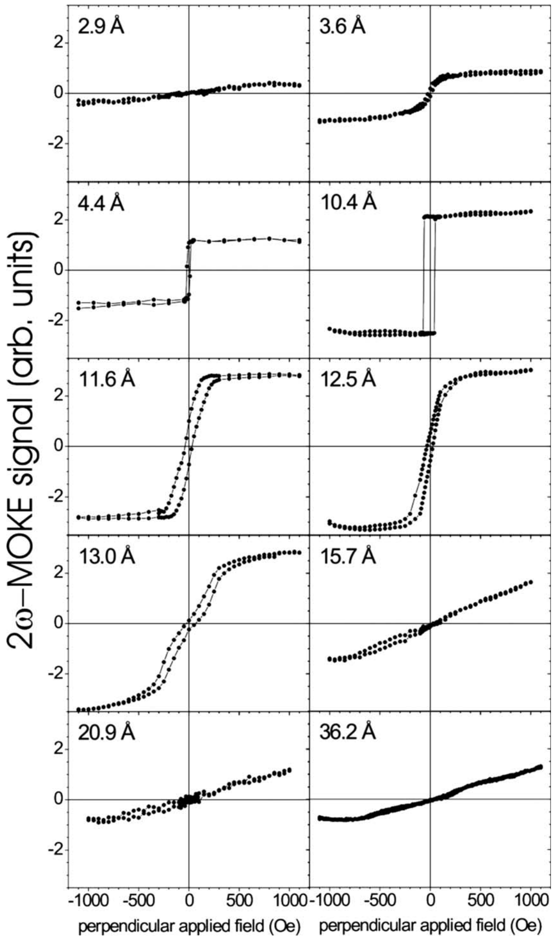

FIG. 2. Thickness dependence of the hysteresis loops of Co films deposited on a clean Pt(111) surface. The films were grown and measured at 200 K. The magnetic field direction is perpendicular to the film.

In Fig. 2 the hysteresis loops of films grown at low temperatures are shown for perpendicular applied field. For the thinnest films (e.g., $t=2.9$ Å) the loops present almost zero remanence and no clear saturation at the largest applied fields (1000 Oe). This probably corresponds to a paramagnetic state, which would imply that the Curie temperature for $t=2.9$ Å is lower than 200 K. Notice that for such low coverages, the presence of superparamagnetic behavior cannot be completely excluded *a priori*. In fact, one could, in principle, have an inhomogeneous, nonpercolating morphology at the early stages of the growth. Nevertheless, such an islandlike film structure seems improbable since the growth mode has been shown to be two-dimensional (layer-by-layer like) for 2–3 Co monolayers.[40] The reason for the two-dimensional growth for such small thickness appears to be due to the presence of strain at the interface between the Co overlayer and the Pt(111) surface, which hinders the formation of straight steps.[40] For $t=3.6$ Å the onset of PMA is clearly reflected by the square shape of the magnetization loop, which show high remanent magnetization, and reach saturation at fields on the order of 40 Oe, a value similar to the coercivity. Beyond $t=11.6$ Å the magnetic behavior starts to change: the remanence decreases and the saturation field increases, becoming much larger than the corresponding coercive field. For even larger thicknesses the perpendicular direction becomes a hard magnetic axis. For example, the 15.7 Å film could not be saturated at the largest attainable fields. This reflects the expected off-plane to in-plane SRT as a function of increasing thickness. As a result, the polar MOKE signals decrease at the largest fields. As previously reported,[22] this behavior can be understood as a more or less continuous reorientation of the easy axis which does not take place as abruptly as for films grown at room temperature. For low-temperature Co/Pt(111) films, the SRT actually extends over a larger thickness range showing an intermediate state where the orientation of the easy axis is canted with respect to the surface normal. A more detailed report and discussion of the in-plane and out-of-plane hysteresis loops of Co/Pt(111) films grown at 300 and 200 K is given in Ref. 22.

B. Hydrogen preadsorbed films

In order to prepare the films with interface H adsorption, the clean Pt(111) surface was exposed to H prior to deposition of the Co layer by introducing a controlled clean H_2 atmosphere of pressure 5.1×10^{-8} mbar. This procedure was

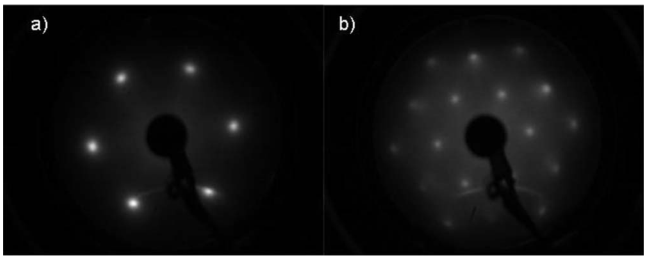

FIG. 3. LEED patterns of a 29 Å Co film grown at 200 K after H preadsorption. The primary electron beam energy is (a) 122.5 eV and (b) 252 eV.

realized during a limited time by completing approximately a 20 Langmuir total exposure. The substrate temperature was kept there at 200 K. In this way only the surface preadsorbed hydrogen interacts with the deposited Co atoms. The quality of the Co-film growth with H preadsorption is similar or better than that of the unexposed films grown at the same temperature ($T=200$ K). This remarkable result is evidenced by the sharp spots and the very low diffuse intensity of the LEED patterns shown in Fig. 3. Concerning the magnetic behavior, the hysteresis loops show no sign of PMA. Instead, a well-defined in-plane magnetization is observed already for thicknesses as small as $t=2.9$ Å. The almost saturated squarelike shape of the in-plane magnetization loops [Fig. 4(a)] contrasts with the hard-axislike shape of the out-of-plane ones [Fig. 4(b)].

It is interesting to observe that the lowest thickness at which ferromagnetism is detected is practically the same in all the experiments [i.e., 3.6 Å for Co films grown on clean Pt(111) and about 2.9 Å for the films grown after H exposure]. This suggests that H adsorption does not result in any magnetic dead layers. Notice however that the hysteresis curves in Fig. 4(a) show a nonmonotonous dependence of the coercive field on film thickness. This could reflect changes in the dominant mechanisms of magnetization reversal involving DW movement and rotation of the spins.

Comparing the hysteresis loops along the easy axes in Fig. 2 (perpendicular to the film for clean Pt substrate) and Fig. 4(a) (in-plane for H-preadsorbed Pt substrate) one observes some remarkable quantitative differences. This reflects the low dimensionality of the magnetic material (confinement effect). In fact, the extension and motion of the magnetic-domain walls associated to magnetization reversal should very different in both cases since one of them concerns the extended film plane while the other the very reduced dimension in the perpendicular direction (one or two atomic layers). Nevertheless, strictly speaking, one cannot completely exclude the possibility that the different behaviors could also be partly a consequence of some differences in the film morphology.

It is interesting to observe that the coercive fields for in-plane magnetization are much larger (about a factor four) than those corresponding to unexposed films, reaching values of up to 200 Oe. In sum, the results shown in Fig. 4 and, in particular, the contrast with Fig. 2, demonstrate the crucial role of the CoPt interface on the development of PMA, and the possibility of controlling this remarkable effect by manipulating the film-substrate interface.

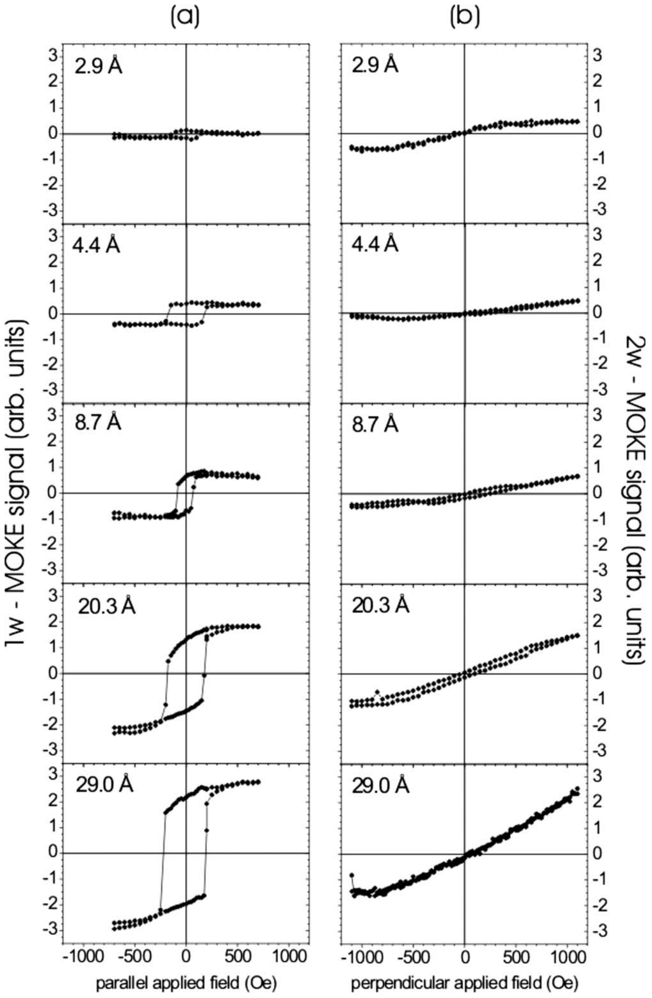

FIG. 4. Thickness dependence of the magnetic hysteresis loops of Co films grown and measured at 200 K after exposing the Pt(111) substrate to 20 Langmuirs of H_2. The applied magnetic field is (a) within the surface plane and (b) perpendicular to the surface.

There are a number of experimental indications that the changes in the magnetic anisotropy observed in this work are not the consequence of important changes in the film structure. Indeed, the structure of ultrathin Co films on Pt(111) have already been extensively studied in a number of previous works.[22,33,34] These studies show that low-temperature growth improves of the quality of the Co/Pt(111) film as compared to the room-temperature case. Lowering the substrate temperature by about 100 K yields a better hcp stacking by decreasing the number of faults.[22] Intermixing effects become important only for temperatures well above room temperature, where the formation of interface alloys causes changes in the MAE and Kerr-effect enhancements.[32–35] The improved quality of the hcp growth after H preadsorption suggests that the suppression of PMA is not due to a structural effect. Moreover, taking into account that the roughness of the films obtained at low temperatures is small, we do not expect any significant dipolar contribution to the MAE due to roughness.[41]

The above discussion suggests, that the main reasons for the strong suppression of PMA should have an electronic origin. Several independent recent studies have provided evidence of the fact that the PMA of Co/Pt(111) is intimately related to the properties of the Co/Pt interface. Electronic calculations show that no important reduction in the interface Co moment takes place.[42] Moreover, the Pt atoms at the interface develop an induced ferromagnetic moment of about $0.20-0.25\mu_B$.[43] In Refs. 13 and 15 the origin of PMA of Co/Pt(111) has been related to the hybridization between Pt and Co. A similar behavior has also been observed in the case of a Pd(111) substrate.[12] The importance of the interface MAE and its modifications upon H adsorption on the magnetoanisotropic behavior of Co/Pt(111) films can be estimated by looking at the critical thickness t_c beyond which the film shows a stable in-plane magnetization. From Fig. 2, we derive $t_c(\text{clean}) \simeq 13$ Å for the unexposed films whereas from Fig. 4(a) we obtain about $t_c(\text{H}) \simeq 3$ Å for the exposed film. Therefore, the ratio between the critical thicknesses $[t_c(\text{H})/t_c(\text{clean}) \simeq 0.2]$ for the off-plane to in-plane reorientation transitions with and without H preadsorption provides a rough estimate of the importance of the effect of H interface adsorption on the stability of the perpendicular magnetization direction.

Interactions between the adsorbed gas and the Co and Pt atoms at the interface are expected to produce significant changes in their electronic structure and as a consequence changes in the MAE. The effect of adsorbates of the film electronic structure has been experimentally quantified by photoemission studies showing important relative changes in the occupied electronic states at the Fermi level after O and H adsorptions.[36,44] As already mentioned, a reduction in the density of electronic states at the Fermi level directly affect the properties of band ferromagnetism which should be accompanied by changes in the MAE.[37,38] These photoemission results are consistent with the present modifications in the direction of the easy axis by means of interface manipulation. A more detailed discussion of the role of the interfaces on the MAE from the point of view of theory is found in the second part of this work.

To conclude this section, it is interesting to discuss the effects of adsorbates on the coercive filed since it provides information on the mechanisms of nucleation and propagation of DWs occurring in magnetization reversal process.[45–49] On the one side, magnetic defects may serve as centers for DW pinning and should thus tend to increase the coercive field. On the other side, as any defect, adsorbates should favor the nucleation of inverse-magnetized domains and would tend to decrease the coercivity. The actual trend on the coercive force depends therefore on the dominant magnetization reversal process (nucleation or propagation of DWs). Our results indicate that the effect of roughness on the coercivity is relatively small since the room-temperature films which show a larger roughness does not show any higher coercive fields than the films grown at 200 K. The adsorption of H, however, does increase the coercive force, which is probably due to an increase in the DW pinning. This interpretation is consistent with the fact that the shape of hysteresis loops of films grown after H adsorption deviate more from a square than those of films grown on clean surfaces. Abrupt magnetization reversals are likely to happen mostly when the propagation field is smaller than the nucleation field since in this case the DW can easily sweep across the whole layer as soon as it nucleates. In contrast, a distribution of pinning-center strength corresponds to a progressive propagation of the DWs and to smoother hysteresis loops. Notice that pinning can have its origin directly at the adsorbate atoms, which constitute nonmagnetic or reduced magnetic centers, or at the structural defects they might induce in the magnetic film.

III. ELECTRONIC CALCULATIONS

The purpose of this section is to investigate the magnetoanisotropic properties of Co films on Pt(111) from a theoretical perspective in order to characterize microscopically the interfaces responsible for PMA and to quantify its dependence on various possible adsorbate-induced modifications in the local magnetic moments. Taking into account that spin-orbit (SO) interactions are very sensitive to the details of the electronic spectrum, we perform accurate self-consistent calculations for each orientation of the magnetization $\vec{M}$ and derive the MAE in a nonperturbative way as the difference between electronic energies.[12,50–53] This is also important in order to investigate the correlation between the spin-polarized density distribution and the MAE.

We consider a tight-binding Hamiltonian given by the sum of three terms: the interatomic hopping term H_0, the Coulomb interaction term H_C, and the SO coupling term H_{SO}. For each magnetization direction δ the local densities of electronic states (DOSs) $\rho^{\delta}_{l\alpha\sigma}(\varepsilon)$ at layer l, orbital α, and spin σ are determined self-consistently by treating H_0, H_C, and H_{SO} on the same footing.[12,50–53] The δ-dependent energy is then calculated as $E_\delta = E^{\text{DD}}_\delta + E^{\text{MC}}_\delta$, where E^{DD}_δ refers to the dipole interaction and $E^{\text{MC}}_\delta = \Sigma_l E^{\text{MC}}_\delta(l)$ to the electronic or magnetocrystalline (MC) energy. The latter can be written as the sum of layer-resolved contributions

$$E^{\text{MC}}_\delta(l) = \sum_{\alpha\sigma} \left[\int_{-\infty}^{\varepsilon_F} \varepsilon \rho^{\delta}_{l\alpha\sigma}(\varepsilon) d\varepsilon - E^{\text{dc}}_{l\alpha\sigma} \right], \qquad (1)$$

where $E^{\text{dc}}_{l\alpha\sigma}$ is the double counting correction. Finally, the MAE per Co atom is given by the energy change $\Delta E_{\delta\gamma} = (E_\delta - E_\gamma)/m$ associated with a change in the orientation of $\vec{M}$. Here we consider the in-plane magnetization direction $\gamma = x$, along a nearest-neighbor bond, for example, $[1\bar{1}0]$, and the film normal $\delta = z$ along [111]. The electronic DOSs $\rho_{l\alpha\sigma}(\varepsilon)$ are computed by using Haydock-Heine-Kelly's recursion method.[54] The number of levels K of the continued fraction expansion of the Green's functions is increased systematically until the calculated MAEs become independent of K. All the recursion coefficients are determined exactly for the semi-infinite configuration of the Co film on the Pt substrate without any spurious boundary effects. The self-consistent equations for the spin-polarized density distribution are solved with an accuracy ε, which is high enough to ensure that the small energy differences involved in the MAEs can be determined reliably (typically $\varepsilon < 10^{-10}$ electrons per orbital). Within the model, the estimated accuracy of the calculated MAEs is of the order 10^{-3} meV or better.[12,53]

The parameters used for the calculations are determined as in Ref. 12. The intra-atomic d-electron exchange integrals

J yield the proper magnetic moment and exchange splitting in the solid ($J_{\mathrm{Co}}=0.76$ eV). For Pt J is obtained from local spin-density calculations ($J_{\mathrm{Pt}}=0.52$ eV).[55] The SO-coupling constants are $\xi_{\mathrm{Co}}=88$ meV and $\xi_{\mathrm{Pt}}=600$ meV.[56] Concerning the film structure we assume for simplicity an unrelaxed bulklike Pt(111) substrate and a perfect epitaxial layer-by-layer Co-film growth. The distance between the Co an Pt atoms at the interface is approximated by the average $d_{\mathrm{CoPt}}=(d_{\mathrm{Co}}+d_{\mathrm{Pt}})/2$ of the bulk value, which is close to the experimental observations.[57] While the assumption of epitaxial growth is an appealing theoretical idealization, it is also true that real Co films show significant deviations from perfect epitaxy already for the smallest thicknesses. Therefore, in order to quantify the effect of vertical and lateral strain we have performed calculations for representative examples by varying the interlayer and lateral distances in the Co film and at the interfaces. We observe that lattice relaxations involving 3–5 % vertical and up to 9% lateral strain do not affect the main trends and conclusions. As it will be discussed below, this is a consequence of the robustness of the Co magnetic moments. Finally, one should mention that the local DOSs, as well as the spin- and orbital-polarized charge densities, are calculated self-consistently in all Co layers, including four layers of the Pt substrate.

The MAE and the resulting orientation of easy and hard axes are known to be very sensitive to the local atomic and magnetic environment, which can be modified by introducing surface and interface adsorbates (e.g., O, H, or CO). In order to investigate the microscopic origin of the perpendicular anisotropy of Co films on Pt(111) we have varied systematically the exchange integral or Stoner parameter J_l at the atoms of the relevant layers l, which controls the corresponding local magnetic moments. For an m-layer film the interesting cases are $J_{\mathrm{Co}(1)}$ at the uppermost Co-surface layer $l=1$, $J_{\mathrm{Co}(m)}$ at the Co layer in contact with the substrate, and $J_{\mathrm{Pt}(m+1)}$ at the Pt interface layer $l=m+1$. In this way the effects of adsorbates on the magnetic moments of the surface and interface layers of the film can be simulated and the resulting changes in the orientation of the magnetization can be quantified. As it will be discussed below, modeling the interactions locally provides new insights into the microscopic origin of perpendicular magnetic anisotropy.

In the following results are given for the MAE per atom defined as $\Delta E=E_x-E_z$ so that positive (negative) values of ΔE correspond to a perpendicular (in-plane) easy axis. First, we consider the film average $\Delta E=(1/m)\Sigma_l^N \Delta E(l)$, which determines the easy axis ($N=m+4$). Notice that the sum takes into account the important contributions from the substrate. In practice, including four layers below the interface (i.e., $N=m+4$ for an m-layer film) yields a very good convergence. In addition we focus on the surface and interface MAEs that are derived from the local contributions $\Delta E(l)=E_x(l)-E_z(l)$ [see Eq. (1)]. Besides the local term $\Delta E(1)$ of the uppermost layer, we consider the *surface* MAE given by the sum $\Delta E^S=\Delta E(1)+\Delta E(2)$ of the contributions of the two uppermost Co layers and the Co-Pt *interface* MAE given by the sum $\Delta E^I=\Delta E(m)+\Delta E(m+1)$ of the contributions of the Co and Pt layers that are in contact. The definition of interface and surface anisotropies is somewhat arbitrary particularly in an ultrathin film. However, one can show, in agreement with previous investigations,[12] that the interface MAEs defined in this way preserve their identity and remain approximately independent of m even for the thinnest films. The robustness of the interface MAE in a variety of film configurations suggests that the relevant magnetic interactions between Co and Pt are essentially short ranged. Finally, it is often useful to focus the analysis on the most important magnetocrystalline contribution ΔE^{MC} to the anisotropy energy $\Delta E=\Delta E^{\mathrm{MC}}+\Delta E^{\mathrm{DD}}$, where ΔE^{DD} refers to the dipolar contribution.

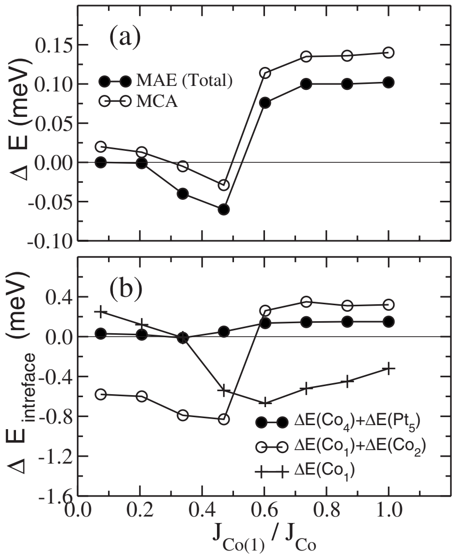

FIG. 5. MAE of $\mathrm{Co}_4/\mathrm{Pt}(111)$ films as a function of the exchange integral $J_{\mathrm{Co}(1)}$ of the Co surface atoms. $J_{\mathrm{Co}}=0.76$ eV corresponds to Co bulk. (a) Total anisotropy energy $\Delta E_{xz}=E_x-E_z=\Delta E_{xz}^{\mathrm{MC}}+\Delta E_{xz}^{\mathrm{DD}}$ (full circles) and magnetocrystalline anisotropy energy $\Delta E_{xz}^{\mathrm{MC}}$ (open circles). (b) CoPt interface MAE $\Delta E_{\mathrm{CoPt}}^{I}=\Delta E_{\mathrm{Co}}^{\mathrm{MC}}(4)+\Delta E_{\mathrm{Pt}}^{\mathrm{MC}}(5)$ (full circles), surface MAE $\Delta E^S=\Delta E_{\mathrm{Co}}^{\mathrm{MC}}(1)+\Delta E_{\mathrm{Co}}^{\mathrm{MC}}(2)$ (open circles), and uppermost-layer contribution $\Delta E_{\mathrm{Co}}^{\mathrm{MC}}(1)$ (crosses).

A. Tuning the magnetic moments at the Co surface atoms

In Figs. 5 and 6 results are given for the MAE of a four-layer Co film on Pt(111) as a function of the surface exchange integral $J_{\mathrm{Co}(1)}$. First of all, for the unperturbed film having $J_{\mathrm{Co}(1)}=J_{\mathrm{Co}}$ one obtains a perpendicular orientation in agreement with experiment [see Fig. 5(a)]. Comparing the different local and interface terms [Fig. 5(b)] one concludes that the perpendicular easy axis is stabilized by the positive surface and interface anisotropies ΔE^S and ΔE^I. Notice, however, that the surface layer $l=1$ alone would favor the in-plane direction since $\Delta E(1)<0$. A similar result has already been reported for $\mathrm{Co}_m/\mathrm{Pd}(111)$.[12] The calculations as a function of the surface exchange integral $J_{\mathrm{Co}(1)}$ show that the MAE is actually quite robust. Indeed, a reduction in $J_{\mathrm{Co}(1)}$ does not change the easy axis, which remains off-plane except for very small values $J_{\mathrm{Co}(1)}/J_{\mathrm{Co}}\leq 0.5$ (see Fig. 5). Notice, moreover, that for $J_{\mathrm{Co}(1)}/J_{\mathrm{Co}}\geq 0.6$ the surface and interface anisotropy energies remain practically unchanged. In contrast, for $J_{\mathrm{Co}(1)}/J_{\mathrm{Co}}\leq 0.5$ an important reduction in ΔE is observed leading to a slight stabilization of the in-plane di-

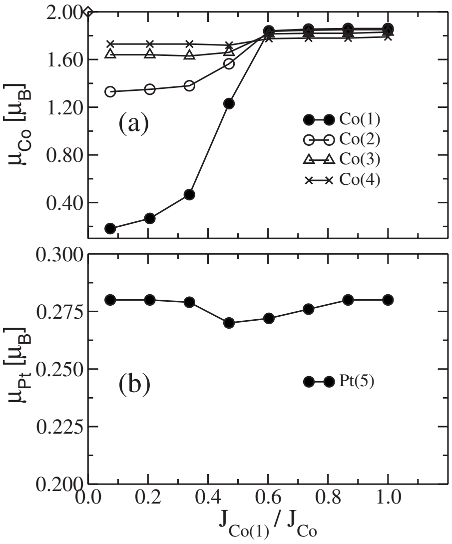

FIG. 6. Local spin plus orbital magnetic moments $\mu(m)$ at the different layers m of a $\mathrm{Co}_4/\mathrm{Pt}(111)$ film as a function of the exchange integral $J_{\mathrm{Co}(1)}$ of the Co surface atoms. $J_{\mathrm{Co}}=0.76$ eV corresponds to Co bulk. Co(m) refers to the mth Co layer, $m=1$ to the surface layer, and Pt(5) to the uppermost substrate layer.

rections. This is mainly due to an abrupt change in sign of ΔE^S. As expected, the CoPt interface MAE ΔE^I is not much affected by manipulations of the film surface.

The changes in the MAE can be correlated with the dependence of the local magnetic moments as a function of $J_{\mathrm{Co}(1)}$ (see Fig. 6). First, for $J_{\mathrm{Co}(1)}$ close to J_{Co}, the nearly saturated Co spin moments are not significantly modified. Only when $J_{\mathrm{Co}(1)}$ is reduced below approximately $J_{\mathrm{Co}}/2$ an important reduction in the local moments at the uppermost two layers is obtained. This explains qualitatively the robustness of the MAE for $J_{\mathrm{Co}(1)}/J_{\mathrm{Co}}>0.5$ and the change in sign of the surface anisotropy $\Delta E(\mathrm{Co}_1)+\Delta E(\mathrm{Co}_2)$ for $J_{\mathrm{Co}(1)}/J_{\mathrm{Co}}\leq 0.5$ shown in Fig. 5(b). In contrast the moments at the deeper layers $l\geq 3$, in particular, at the CoPt interface, are only slightly modified. Consequently, the electronic structure and MAE at the CoPt interface are much less affected. This indicates that the reorientation transition observed after the deposition of H on the Pt(111) substrate is not due to a modification in the magnetic behavior of the Co surface layer. Notice that a strong reduction in the magnetic moments at the surface layers, as obtained for $J_{\mathrm{Co}(1)}/J_{\mathrm{Co}}\leq 0.5$, would imply an important decrease in the total film magnetization, which is not observed in experiment.

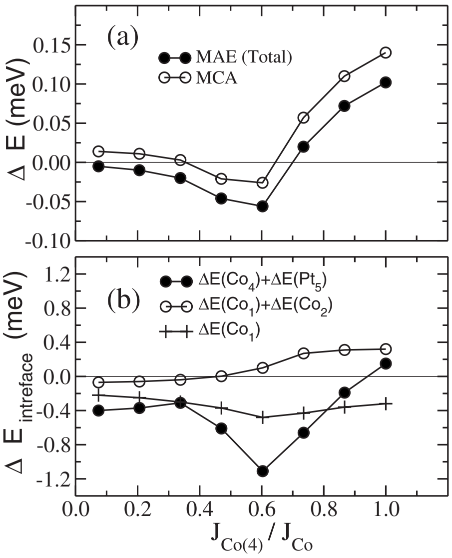

FIG. 7. MAE of $\mathrm{Co}_4/\mathrm{Pt}(111)$ films as a function of the exchange integral $J_{\mathrm{Co}(4)}$ of the Co atoms at the CoPt interface. (a) Total anisotropy energy ΔE_{xz} (full circles) and magnetocrystalline anisotropy energy $\Delta E_{xz}^{\mathrm{MC}}$ (open circles). (b) CoPt interface MAE $\Delta E^I_{\mathrm{CoPt}}$ (full circles), surface MAE ΔE^S (open circles), and uppermost-layer contribution $\Delta E^{\mathrm{MC}}_{\mathrm{Co}}(1)$ (crosses).

B. Tuning the Co moments at the CoPt interface

The situation is qualitatively different when the effective exchange interaction $J_{\mathrm{Co}(m)}$ at the *interface* Co atoms is modified. The corresponding results for the MAE and local magnetic moments of a four-layer Co film on Pt(111) are shown in Figs. 7 and 8. In this case the local magnetic moments of the Co interface layer $\mu_{\mathrm{Co}(4)}$ and of the adjacent Pt layer $\mu_{\mathrm{Pt}(5)}$ both decrease quite rapidly with decreasing $J_{\mathrm{Co}(4)}$ (see Fig. 8). As a result the interface anisotropy energy $\Delta E^I_{\mathrm{CoPt}}$, which is positive and thus favors the off-plane orientation for $J_{\mathrm{Co}(4)}/J_{\mathrm{Co}}=1$, is strongly reduced and changes sign already for $J_{\mathrm{Co}(4)}/J_{\mathrm{Co}}\simeq 0.9$ [see Fig. 7(b)]. Moreover, $\Delta E^I_{\mathrm{CoPt}}$ continues to decrease for $J_{\mathrm{Co}(4)}/J_{\mathrm{Co}}<0.9$ (larger $|\Delta E^I_{\mathrm{CoPt}}|$) which tends to stabilize more and more the in-plane magnetization direction. Consequently, the easy axis switches to in-plane even if the reduction in $J_{\mathrm{Co}(4)}$ is relatively small. As expected, the contributions of the surface layers $\Delta E^{\mathrm{MC}}_{\mathrm{Co}}(1)$ and $\Delta E^{\mathrm{MC}}_{\mathrm{Co}}(2)$ are not much affected by manipulations at the CoPt interface although a reduction and

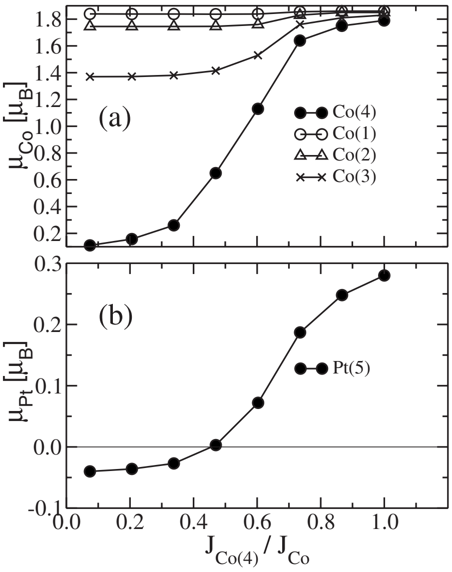

FIG. 8. Local orbital plus spin magnetic moments $\mu(m)$ at the different layers m of a $\mathrm{Co}_4/\mathrm{Pt}(111)$ film as a function of the exchange integral $J_{\mathrm{Co}(4)}$ of the Co atoms at the CoPt interface. See the caption of Fig. 6.

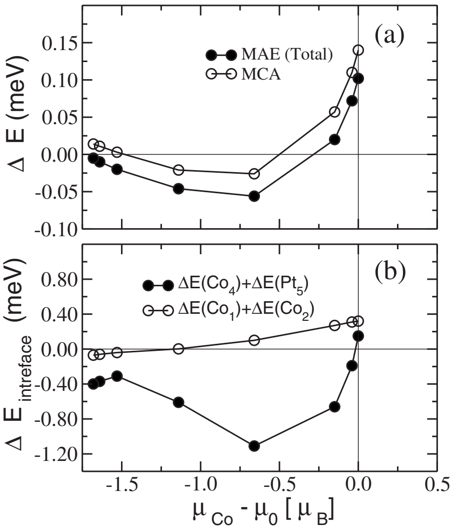

FIG. 9. Magnetic anisotropy energy (MAE) of $Co_4/Pt(111)$ films as a function of the magnetic moment $\mu_{Co}(4)$ of the Co layer $m=4$ at the CoPt interface. The results are obtained by varying the exchange integral $J_{Co(4)}$ of the Co atoms at the CoPt interface, as in Fig. 7. $\mu_0=1.79\mu_B$ refers to the Co moment $\mu_{Co}(4)$ obtained for $J_{Co(4)}$ equal to the bulk value J_{Co}. (a) Total anisotropy energy $\Delta E_{xz}=\Delta E_{xz}^{MC}+\Delta E_{xz}^{DD}$ (full circles) and magnetocrystalline anisotropy energy ΔE_{xz}^{MC} (open circles). (b) CoPt interface MAE ΔE_{CoPt}^{I} (full circles) and surface MAE ΔE^{S} (open circles).

change in sign of ΔE^{S} are observed for very small $J_{Co(4)}/J_{Co}\leq 0.4$. This reduction in the surface MAE actually enhances the relative importance of the CoPt interface MAE.

A complementary perspective to the SRT is given in Fig. 9 where the MAE is plotted as a function of the Co interface moment $\mu_{Co(4)}$. Here we observe that a reduction in $\mu_{Co(4)}$ of only $0.2\mu_B(\simeq 10\%)$ is enough to switch the magnetization direction within the film. This contrasts remarkably with the trends found at the surface, where the easy axis remains off-plane even for $\mu_{Co(1)}$ as small as $0.5\mu_B$. The calculations thus confirm the conclusion of the experimental study that the SRT induced by H preadsorption on the substrate is intrinsically related to a modification in the magnetic properties of the CoPt interface.

The correlation between Co and Pt interface moments is central to understanding the microscopic mechanism responsible for the perpendicular magnetization direction. As shown in Fig. 10, $\mu_{Pt(5)}$ decreases rapidly with decreasing $\mu_{Co(4)}$, and it is in fact this reduction in the induced Pt moments what drives the change in sign of ΔE_{CoPt}^{I} and the magnetization reorientation. To investigate the matter further we have performed self-consistent calculations on $Co_4/Pt(111)$ by setting the spin-orbit interaction at the Pt atoms $\xi_{Pt}=0$. In this case, the values of Co and Pt spin moments are essentially the same as for $\xi\neq 0$. However, the easy axis is now in-plane. One concludes that the Pt magnetic moments, which are induced by the adjacent Co moments and the associated spin-orbit interactions at the interface Pt atoms are the most important microscopic source of the PMA observed in $Co_m/Pt(111)$. A similar effect has already been observed at CoPd interfaces.[12] Further details are discussed in the following section.

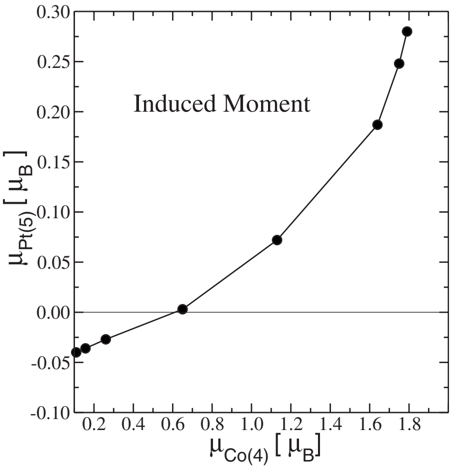

FIG. 10. Local orbital plus spin magnetic moment $\mu_{Pt}(5)$ induced at the Pt atoms of the CoPt interface in a $Co_4/Pt(111)$ film as a function of the Co moment $\mu_{Co}(4)$ at the interface Co layer. The results are obtained by varying the exchange integral $J_{Co(4)}$ of the interface Co atoms.

C. Tuning the Pt moments at the CoPt interface

In Figs. 11 and 12 the MAE and local magnetic moments of $Co_4/Pt(111)$ are shown as a function of the exchange integral $J_{Pt(5)}$ at the Pt interface atoms. Remarkably, $J_{Pt(5)}$ has no qualitative and little quantitative effect on these properties. While this simple, almost boring results could have been anticipated in some cases [e.g., ΔE_{Co}^{S} and the Co surface moments were expected to be essentially independent of $J_{Pt(5)}$] it actually hides some very interesting conclusions. The interface MAE shows a monotonous and significant de-

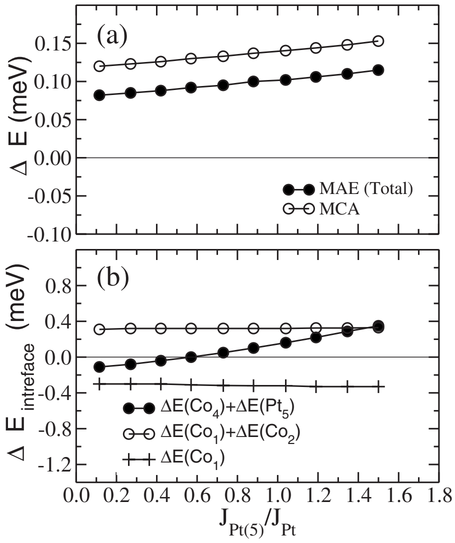

FIG. 11. MAE of $Co_4/Pt(111)$ films as a function of exchange integral $J_{Pt}(5)$ of the Pt atoms at the CoPt interface. $J_{Pt}=0.60$ eV corresponds to Pt bulk. (a) Total anisotropy energy $\Delta E_{xz}=\Delta E_{xz}^{MC}+\Delta E_{xz}^{dip}$ (full circles) and magnetocrystalline anisotropy energy ΔE_{xz}^{MC} (open circles). (b) CoPt interface MAE ΔE_{CoPt}^{I} (full circles), surface MAE ΔE^{S} (open circles), and uppermost-layer contribution $\Delta E_{Co}^{MC}(1)$ (crosses).

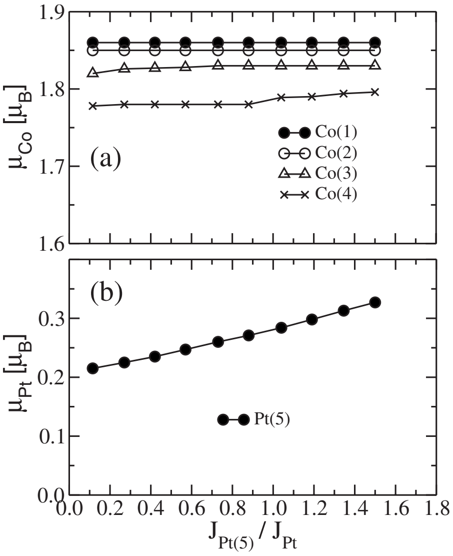

FIG. 12. Local orbital plus spin magnetic moments $\mu(m)$ at the different layers m of a Co$_4$/Pt(111) film as a function of the exchange integral $J_{Pt(5)}$ of the Pt atoms at the CoPt interface.

crease from $\Delta E^I_{CoPt}=0.2$ meV for $J_{Pt(5)}=J_{Pt}$ to $\Delta E^I_{CoPt}=0.0$ meV for $J_{Pt(5)}=0.5J_{Pt}$. This is a consequence of the reduction in the Pt moments [see Fig. 12(b)]. In fact, it is well known that the exchange interaction at the Pt atoms is responsible for an important enhancement of the magnetic susceptibility of Pt. The present calculations show that $\mu_{Pt(5)}$ decreases with decreasing $J_{Pt(5)}$ from $\mu_{Pt(5)}=0.28\mu_B$ for $J_{Pt(5)}=J_{Pt}$ to $\mu_{Pt(5)}=0.21\mu_B$ for $J_{Pt(5)}=0$. Remarkably, the induced Pt moments at the interface do not vanish even for $J_{Pt(5)}=0$. In other words, the proximity of the Co induces the essential part of the Pt moment. Notice that the characteristic robustness of the Co moments holds even for the layer $i=4$ in contact with substrate. For these reasons [robustness of $\mu_{Co(4)}$ and significant $\mu_{Pt(5)}$] the interface magnetic anisotropy energy, which always favors the off-plane direction, is not much affected by the reduction in $J_{Pt(5)}$. These results are consistent with those of the previous section, where a reorientation transition is observed, since in that case the reduction in the Pt moments is much stronger (see Fig. 10). Moreover, in the previous calculations (Sec. III B) the contribution of the Co interface atoms to the MAE, which also favors the off-plane direction [$\Delta E^{MC}_{Co}(4)>0$], is also affected by the reduction in the interface Co moments (see Fig. 8).

In sum, the induced Pt moments are not very sensitive to the value of the intra-atomic Pt exchange interactions although they are certainly enhanced by them. The Pt local moments result dominantly from the hybridization of Pt with the spin-polarized Co layer. Let us recall that the Pt moments are at the origin of the SO interactions that favor the off-plane easy axis since setting $\xi_{Pt}=0$ changes the magnetization direction to in plane. Therefore, any experimental manipulation of the interface that would reduce either the Co moment (and Co exchange splitting) or the hybridization between the Pt substrate and the Co overlayer (e.g., interface adsorbates) should result in a strong reduction in the perpendicular anisotropy, which would favor an off-plane to in-plane SRT.

IV. CONCLUSION

The flexibility of the tight-binding model has been exploited to investigate the role of exchange interactions and magnetic moments on the MAE of Co films on Pt(111) from a local perspective. The main conclusions may be summarized as follows: (i) the calculations reproduce correctly the experimental observed PMA of ultrathin Co films on clean Pt(111). The perpendicular magnetization direction is shown to be stabilized by the contributions of both interfaces (Co vacuum and Co-Pt). (ii) A not too strong reduction in the Stoner parameter J at the uppermost Co layer does not modify the off-plane direction of the magnetization. The same holds for strain effects which have little effect on the Co magnetic moments and on the induced magnetization at the Pt substrate. (iii) The quantitatively important surface MAE $\Delta E^S=\Delta E^{MC}_{Co}(1)+\Delta E^{MC}_{Co}(2)$, which favors the off-plane direction, is not very sensitive to changes in the electronic structure, for example, due to hybridization effects. Therefore, the quantitatively smaller but much more subtle interface MAE $\Delta E^I_{CoPt}=\Delta E^{MC}_{Co}(m)+\Delta E^{MC}_{Pt}(m+1)$ dominates the local environment dependence. (iv) The Pt interface atoms play a crucial role. This has been explicitly demonstrated by calculations setting $\mu_{Pt}=0$ or $\xi_{Pt}=0$, which yield an in-plane easy axis. (v) A reduction in the local magnetic moments at the Co interface atoms or of the coupling between the adjacent Co and Pt layers yields an important quenching of the Pt moments at the interface. This implies a significant decrease in the interface MAE yielding a rotation of the easy axis from off-plane to in-plane. (vi) The magnetic moments of Pt atoms are not very sensitive to changes in the Stoner parameter J of Pt atoms at the interface. Therefore, the origin of the Pt moment is mainly due to the hybridization with the adjacent Co atoms.

The points (i) and (ii) explain the physical mechanisms of the off-plane MAE of clean Co/Pt(111) films while the points (iii) and (vi) reveal the sensitive of the magnetoanisotropic properties to manipulations of the interface. The hybridization with the substrate modifies the electronic structure of the Co interface layer favoring the off-plane direction. In addition, Co induces a moment in the adjacent Pt, which awakens the Pt SOC and favors the off-plane direction. The importance of the Pt magnetic moments has been further investigated by performing calculations of the MAE as a function of the Co(4)-Pt(5) interlayer distance. This allows to explore the idea that interface adsorbates could tend to decouple the magnetic film from the substrate. For vanishing substrate-film hopping (free-standing film) the easy-calculated axis is in-plane and from the previous sections we know that the key to off-plane anisotropy are the moments induced in the Pt. Consequently, if one increases the film-substrate distance the induced Pt moments decrease and the easy axis shifts to in-plane. Moreover, and this might sound counterintuitive at first sight, the calculations also show that decreasing the Co(4)-Pt(5) distance (increasing the hoppings) also yields a SRT from off-plane to in-plane. The reason for this is the increase in the effective local d-band width, and the associated reduction in the Co DOS at the Fermi energy, which quench the Co(4) moment and thus also the Pt(5) moment.

In conclusion, *in situ* surface magneto-optical Kerr-effect experiments show that a remarkable change from perpendicular to in-plane magnetization direction occurs in Co films on Pt(111) as a result of H interface deposition. A stable in-plane easy axis is observed in $\mathrm{Co}_m/\mathrm{H}/\mathrm{Pt}(111)$ already for a Co thickness $m \simeq 1.5$ ML, which implies a complete suppression of stable off-plane magnetization. Layer-resolved self-consistent electronic calculations of the MAE shown that the PMA is quite insensitive to changes in the local magnetic moments at the Co film surface but that it depends crucially on the Co-interface moments, on the Pt-interface moments induced by proximity effects, and on the resulting spin-orbit interactions at the Pt atoms. The experimentally observed magnetization-direction change can be understood to be a consequence of a reduction in the interface-Pt moments due to a reduction in the Co-interface moments or to a decoupling between substrate and film. The dominant role of the interface magnetic anisotropy and the possibility of manipulating it with surfactant interface preadsorption have been demonstrated.

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