PHYSICAL REVIEW B VOLUME 60, NUMBER 1 1 JULY 1999-I

# Magnetic properties of thin films of Co and of (CoPt) superstructures on Pt(100) and Pt(111)

U. Pustogowa and J. Zabloudil
*Center for Computational Materials Science, Gumpendorfer Strasse 1a, A-1060 Vienna, Austria*

C. Uiberacker, C. Blaas, and P. Weinberger
*Institut für Technische Elektrochemie, Technische Universität Wien, Getreidemarkt 9/158, A-1060 Vienna, Austria*

L. Szunyogh
*Center for Computational Materials Science, Gumpendorfer Strasse 1a, A-1060 Vienna, Austria*
*and Department of Theoretical Physics, Technical University Budapest, Budafoki út 8, H-1521, Budapest, Hungary*

C. Sommers
*Institute Physique des Solides, Bâtiment 510, Campus d'Orsay, 91405 Orsay, France*

(Received 6 October 1998)

The magnetic properties of $\mathrm{Co}_n/\mathrm{Pt}(100)$, $\mathrm{Co}_n/\mathrm{Pt}(111)$, $(\mathrm{Co}_{0.5}\mathrm{Pt}_{0.5})_n/\mathrm{Pt}(100)$, $(\mathrm{CoPt})_n/\mathrm{Pt}(100)$, and $(\mathrm{CoPt})_n/\mathrm{Pt}(111)$, $n \leqslant 15$, are investigated using the relativistic spin-polarized screened Korringa-Kohn-Rostoker method. It is found that only the artificial superstructures $(\mathrm{CoPt})_n/\mathrm{Pt}(100)$ and $(\mathrm{CoPt})_n/\mathrm{Pt}(111)$ show a perpendicular magnetic anisotropy beyond $n=10$. For the free surfaces of Co on Pt in the case of the (100) orientation, a multiple reorientation transition below $n=7$ is found, while along (111) such a transition is predicted at about four layers of Co. For the homogeneous, statistically disordered alloy $\mathrm{Co}_{0.5}\mathrm{Pt}_{0.5}$ on Pt(100) the orientation of the magnetization remains in-plane for all $n$ investigated. A comparison to experiment yields interesting insight into aspects of order and disorder, surface segregation, and phase separation frequently encountered in experimental studies of perpendicular magnetism in the Co/Pt system.

[S0163-1829(99)00125-3]

## I. INTRODUCTION

Free surfaces of Co, of $\mathrm{Co}_c\mathrm{Pt}_{1-c}$ alloys, and of artificial superstructures $\mathrm{Co}_n\mathrm{Pt}_m$ on Pt are indeed very interesting from both experimental (for a recent review, see, e.g., Weller,[1] and references therein) and theoretical (see, in particular, Refs. 2–4) points of view, because of technologically relevant discoveries in studies dealing with perpendicular magnetic anisotropy, giant magnetoresistance, and oscillatory exchange coupling. Because of its technological implications in high-density magneto-optical storage media, the Co/Pt system seems to be the candidate of first choice. In this paper a detailed study of the magnetic anisotropy energy of thin films of Co and of Co/Pt superstructures is presented for two different surface orientations, corresponding to Pt(100) and Pt(111) substrates. In particular, the systems $\mathrm{Co}_n/\mathrm{Pt}(100)$, $\mathrm{Co}_n/\mathrm{Pt}(111)$, $(\mathrm{Co}_{0.5}\mathrm{Pt}_{0.5})_n/\mathrm{Pt}(100)$, $(\mathrm{CoPt})_n/\mathrm{Pt}(100)$, and $(\mathrm{CoPt})_n/\mathrm{Pt}(111)$, $n \leqslant 15$, are investigated. By defining a kind of volume independent contribution as well as surface and interface contributions to the magnetic anisotropy energy, a detailed comparison and interpretation of experimental data can be made. It will also be shown that, contrary to common usage, the magnetic anisotropy energy has little in common with the distribution of orbital magnetic moments throughout the magnetic layers.

The paper is organized as follows: in Sec. II a short summary of the computational details is given. Section III deals first with the magnetic anisotropy energy, and then with spin and orbital magnetic moments. Section IV provides a comparison with and microscopic interpretations of available experimental data and is followed by a conclusion summarizing the main aspects of the present study.

## II. COMPUTATIONAL DETAILS

The relativistic spin-polarized version[5] of the screened Korringa-Kohn-Rostoker (SKKR) method[6] for layered systems[7] is applied to calculate self-consistently the electronic structure and the magnetic properties of free surfaces of $\mathrm{Co}_n$ and of an ordered superstructure of $(\mathrm{CoPt})_n$ on Pt(100) and Pt(111), $n \leqslant 15$, whereby all interlayer distances refer to a fcc ''parent lattice''[8] corresponding to the experimental lattice spacing of Pt ($a_0 = 7.4137$ a.u.; no surface or interface relaxations). For each system, i.e., for each $n$, the electronic and magnetic structure of the magnetic configuration corresponding to a *uniform* perpendicular-to-plane orientation of the magnetization in the Co (and Pt) layers is calculated self-consistently using 45 $k_\parallel$ points in the irreducible part of the surface Brillouin zone (ISBZ) and the (nonrelativistic) local-density functional described in Ref. 9. For comparison with the corresponding superstructure, free surfaces of the statistically disordered alloy $(\mathrm{Co}_{0.5}\mathrm{Pt}_{0.5})$ on Pt(100) are also calculated using the coherent-potential approximation for layered systems.[10] In order to reduce the computational effort in this particular case, the semirelativistic version of the SKKR was employed to achieve (charge) self-consistency using the same computational parameters as for all the other cases. In all systems investigated, a buffer of three Pt layers to the Pt substrate was varied self-consistently.

The obtained self-consistent layer-resolved effective potentials and layer-resolved effective magnetization fields are then used to evaluate the band energy contribution $E_b$ to the magnetic anisotropy energy $E_a$,

$$E_a = E_b + E_{\mathrm{dd}}, \tag{1}$$

defined as the energy difference between a *uniform* perpendicular-to-plane and a *uniform* in-plane orientation of the magnetization. In Eq. (1), $E_{\mathrm{dd}}$ is the energetic contribution of the magnetic dipole-dipole interaction to $E_a$. In all cases the band energy contribution $E_b$ was calculated using 990 $k_{\parallel}$ points in the ISBZ. It should be noted that, for $E_a > 0$, an out-of-plane orientation of the magnetization is favored, while for $E_a < 0$ an in-plane orientation has to be expected.

## III. RESULTS

### A. Magnetic anisotropy energies

In Fig. 1 the magnetic anisotropy energy and its contributions are shown for free surfaces of $\mathrm{Co}_n$ on Pt(100) and Pt(111). While in the case of the (100) surface a multiple reorientation transition is seen between three and seven layers of Co, the one between six and seven layers being very distinct, for the (111) surface only at a thickness of four layers of Co a flip over from in-plane to out-of-plane seems likely. For both types of surfaces the magnetic anisotropy energy starts to oscillate for $n \geqslant 11$ with a period of 2, and for $n \geqslant 7$ the contribution from the magnetic dipole-dipole interaction causes a regime of in-plane orientations.

Completely different to the behavior of the magnetic anisotropy energy in Fig. 1 is that of free surfaces of the superstructure $(\mathrm{CoPt})_n$ on these two surfaces of Pt (Fig. 2). First of all, for both types of surfaces an out-of-plane orientation is always favored, which for the (111) surface is almost a factor 10 larger than the one corresponding to the (100) surface. It easily can be seen from Fig. 3 that with respect to the number of layers the shape of the magnetic anisotropy energy for free surfaces of $(\mathrm{Co}_{0.5}\mathrm{Pt}_{0.5})$ on Pt(100) has very little in common with that of the superstructure $(\mathrm{CoPt})_n$ on Pt(100): in the case of the alloy the preferred orientation is always in-plane; the oscillations resemble the various oscillations for the corresponding case of pure Co in Fig. 1. The peaks at $n=2$ and 6 are clearly visible, and at $n=4$ there is only a kind of shoulder present in the alloy case. It should be noted from Fig. 3, however, that with exception of $n=6$ the band energy as well as the magnetic dipole-dipole contribution favor an in-plane orientation of the magnetization.

In all cases investigated the magnetic anisotropy energy per number of repetitions *n*, $E_a/n$ (see Fig. 4), tends to a constant for a sufficiently large *n*, which in the case of the superstructure (CoPt) on Pt(111) is surprisingly large, about 1.4 meV. It can easily be seen from Table I, containing the values of $E_a/n$ for $n=15$, that in all semi-infinite systems investigated the magnetic anisotropy energy is larger by orders of magnitude than comparable bulk values. In a recent evaluation[2] of the magnetic anisotropy energy of bulk $\mathrm{Co}_c\mathrm{Pt}_{1-c}$ alloys, the largest value was found for $c=0.50$, which, however, amounted to only 3 $\mu$eV.

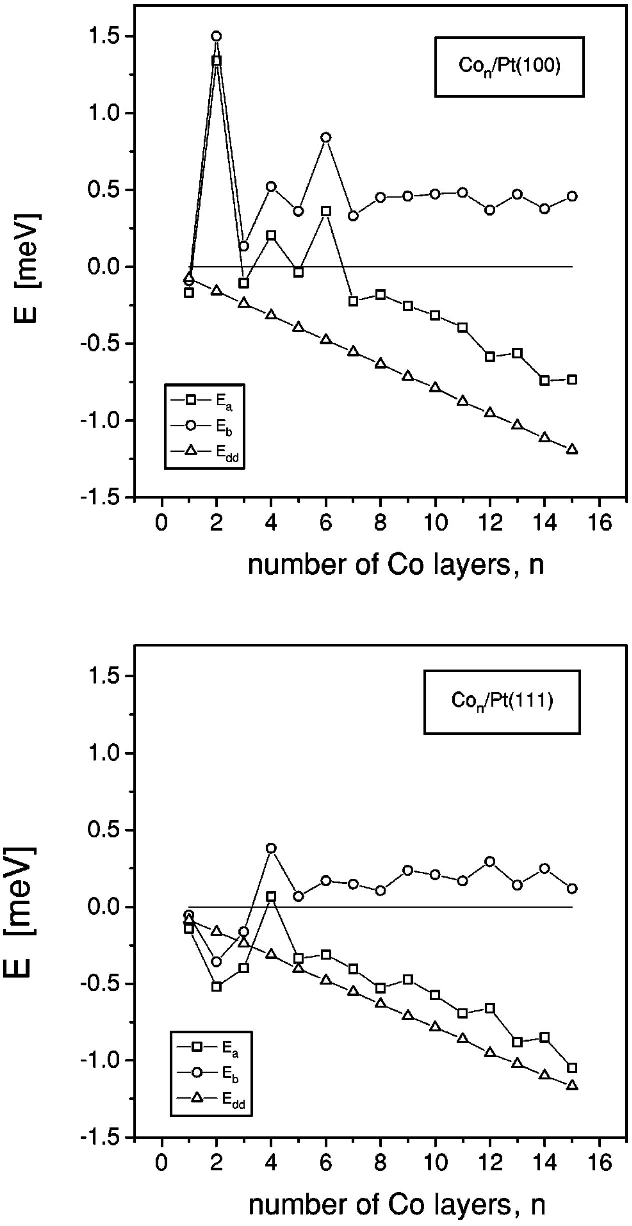

FIG. 1. Magnetic anisotropy energy and its contributions for free surfaces of $\mathrm{Co}_n$ on Pt(100) (top) and Pt(111) (bottom).

In order to demonstrate the fundamental differences between infinite and semi-infinite systems in Fig. 5, the layer-resolved band energies,

$$E_b = \sum_{i=1}^{n} E_i, \tag{2}$$

for $n=15$ are displayed. In this figure the first three layers refer to the Pt buffer, and the remaining layers to the magnetic top. One can easily see that for free surfaces of Co on Pt the (by far) largest contributions to the band energy part of the magnetic anisotropy energy arise from the interface between Pt and Co and from the surface. Somewhat surprising are the contributions from the Pt buffer, i.e., from the induced magnetic effects in the top layers of the substrate. This effect will also be emphasized below in terms of magnetic moments.

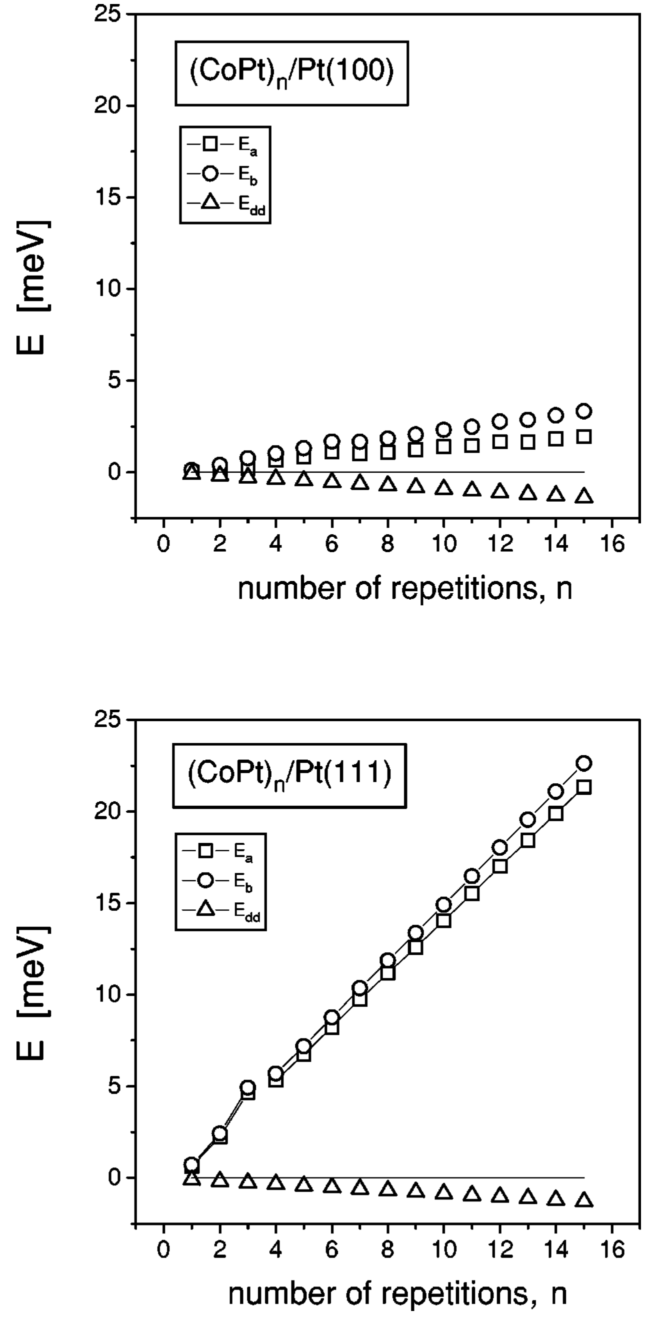

FIG. 2. Magnetic anisotropy energy and its contributions for free surfaces of the superstructure $(\mathrm{CoPt})_n$ on Pt(100) (top) and Pt(111) (bottom).

In the interior of the magnetic multilayers the contributions to $E_b$ vary very little from layer to layer. Excluding, therefore, $m_1$ first layers (the Pt buffer and Co/Pt interface, $m_1=6$) and $m_2$ last layers (the Co/vacuum interface, $m_2=4$), the renormalized contributions from the remaining layers,

$$E_v^b=\frac{1}{n-m_2-m_1}\sum_{i=m_1+1}^{n-m_2} E_i, \tag{3}$$

can be regarded as a volumelike contribution, which, as can be seen from Fig. 5, is very small indeed.

In the alloy case the band energy term is defined as

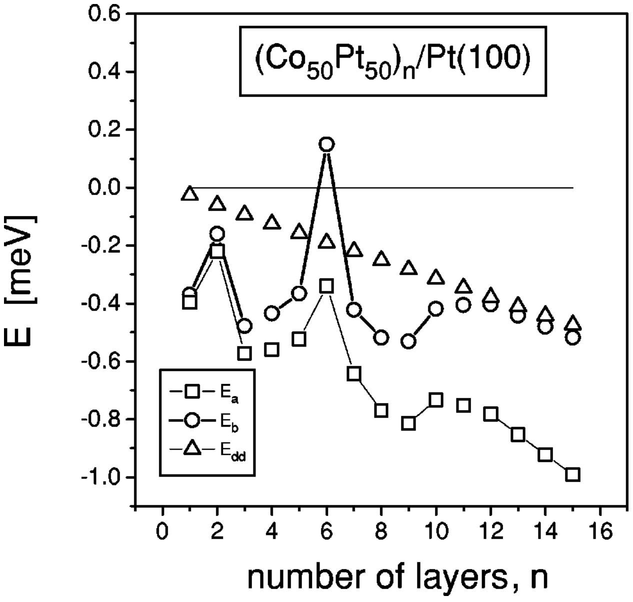

FIG. 3. Magnetic anisotropy energy and its contributions for free surfaces of $(\mathrm{Co}_{0.5}\mathrm{Pt}_{0.5})_n$ on Pt(100).

$$E_b=\sum_{i=1}^{n}\sum_{\alpha=A,B} c_i^{\alpha}E_i^{\alpha}, \tag{4}$$

where $c_i^{\alpha}$ are the concentrations of constituents $A$ and $B$ in the $i$th layer. It should be noted that in Fig. 5 the layerwise band energy contributions for $(\mathrm{Co}_{0.5}\mathrm{Pt}_{0.5})_{15}/\mathrm{Pt}(100)$ are not

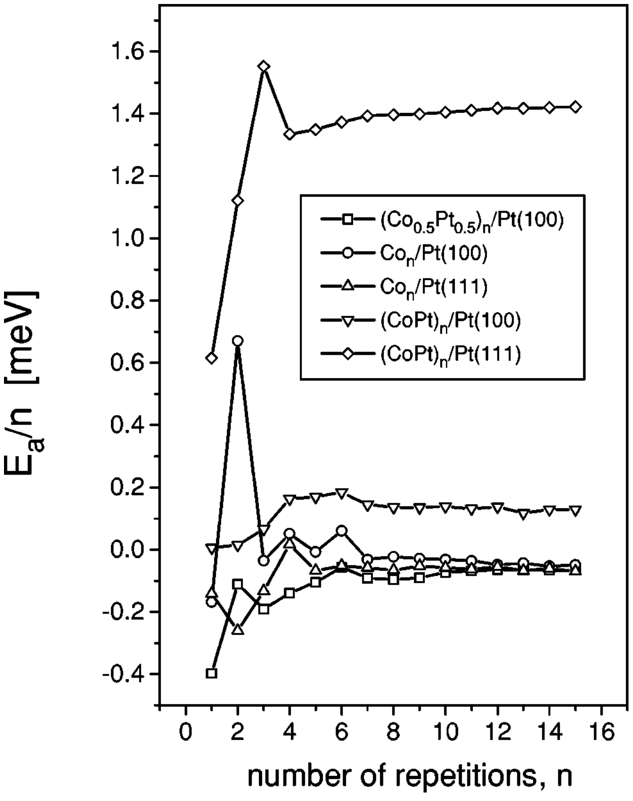

FIG. 4. Magnetic anisotropy energy per repetition for $\mathrm{Co}_n/\mathrm{Pt}(100)$ (circles), $\mathrm{Co}_n/\mathrm{Pt}(111)$ (up triangles), $(\mathrm{CoPt})_n/\mathrm{Pt}(100)$ (down triangles), $(\mathrm{CoPt})_n/\mathrm{Pt}(111)$ (diamonds), and $(\mathrm{Co}_{0.5}\mathrm{Pt}_{0.5})_n$ (squares).

TABLE I. Magnetic anisotropy energies.

| | | $E_a/n$ (meV) | $E_a$ ($\mu$eV) |
|---|---|---|---|
| Infinite (Ref. 2) | $Co_{0.5}Pt_{0.5}$ | | 3 |
| Semi-infinite | Pt(100)/$(CoPt)_{15}$ | 0.129 | |
| | Pt(111)/$(CoPt)_{15}$ | 1.422 | |
| | Pt(100)/$Co_{15}$ | $-0.049$ | |
| | Pt(111)/$Co_{15}$ | $-0.070$ | |
| | Pt(100)/$(Co_{0.5}Pt_{0.5})_{15}$ | $-0.066$ | |

weighted by the concentration $c_i^{\mathrm{Co}} = c_i^{\mathrm{Pt}} = 0.5$. A comparison between the top and bottom rows in Fig. 5 immediately shows that, essentially, the contribution from the interface to the substrate is substantially reduced, whereas the contributions from the surface are—at least in shape—very similar. In all three cases shown in Fig. 5, $E_v^b$ is negative, but rather close to zero. For $Co_n$/Pt(111), e.g., $E_v^b$ is less than $-0.0005$ meV.

Completely different in shape are the layer-resolved band energy contributions for the superstructures of $(CoPt)_{15}$ on either Pt(100) or Pt(111) shown in Fig. 6. Although again the effect of the interface with the Pt substrate and of the surface is clearly visible, now also the interior of the film contributes substantially. In both cases oscillations of $E_i$ with a period of 2 can be seen. While for both surface orientations the contributions from the Pt layers are about the same, namely, about 0.3 meV per Pt layer in the interior of the films, the Co layers behave completely differently: for the (100) orientation the Co contributions are slightly negative and smaller in absolute value than the Pt contributions, whereas along the (111) direction the Co contributions are positive and much larger than those from the Pt layers. Going back now to Figs. 2 and 4, one can state that the preferred perpendicular orientation for $(CoPt)_n$ superstructures on Pt(100) is due to the Pt-like contributions to the band energy term. Furthermore, it is clear from Fig. 6 that the large value of $E_a/n$ for $(CoPt)_n$ superstructures on Pt(111) originates from additional, rather large, positive Co-like contributions.

### B. Magnetic moments

Because the magnetic anisotropy energy of $(CoPt)_n$ superstructures on Pt(111) seems to be so unique, it is interesting to know whether this particular property can be correlated to either the spin-only or orbital (layer-resolved) magnetic moments. In Fig. 7 for one particular case, namely, $(CoPt)_5$, a comparison between Pt(100) and Pt(111) substrates is shown. Easily seen here is a very nice example of the fact that the orbital magnetic moments have little in common with the magnetic anisotropy energy: in the case of a (100) surface the (layerwise) orbital magnetic moments are substantially larger than for a (111) surface, while the shape of the variation with respect to the layers is roughly the same. A similar effect can be seen for the spin-only moments. For the (100) orientation the magnetic moments of the Pt layers are by about $0.1\mu_B$ larger than for the (111) orientation. It is worthwhile to note that in both cases the spin-only magnetic moments of the Pt layers are quite large,

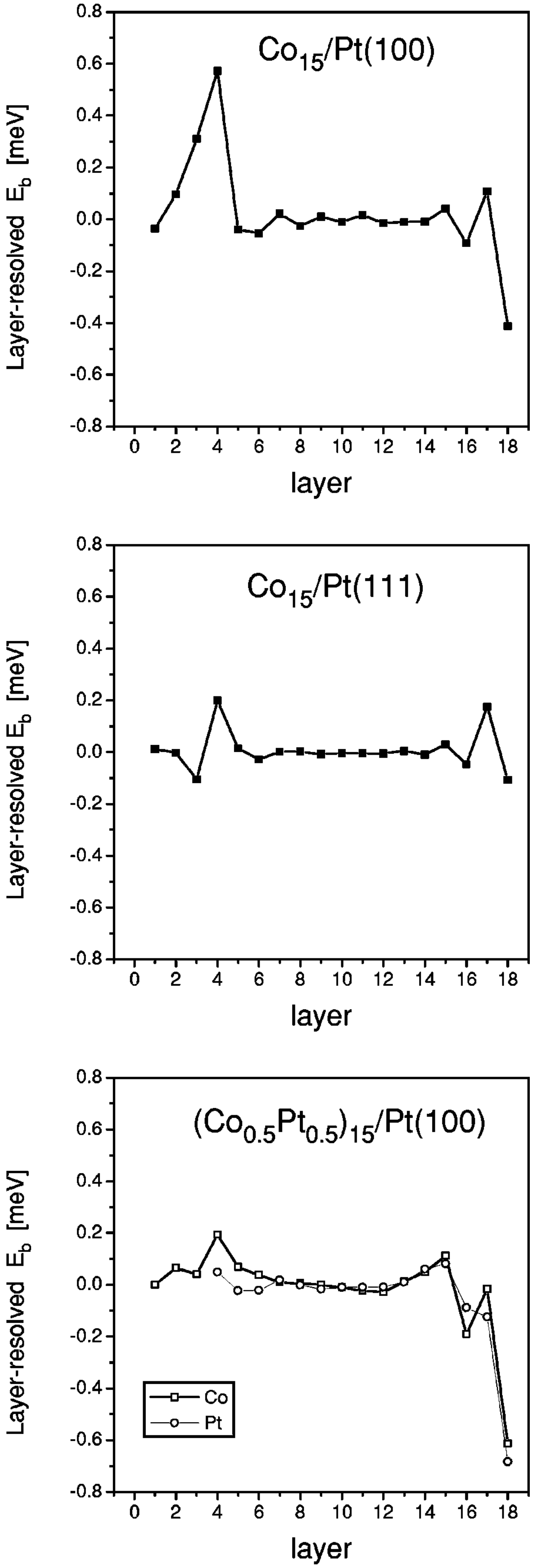

FIG. 5. Layer-resolved band energies for $Co_{15}$/Pt(100) (top) and $Co_{15}$/Pt(111) (middle) and $(Co_{0.5}Pt_{0.5})_{15}$/Pt(100) (bottom). In the alloy case the band energies are *not* weighted by the concentration; the Co contributions are shown as squares, and the Pt contributions as circles.

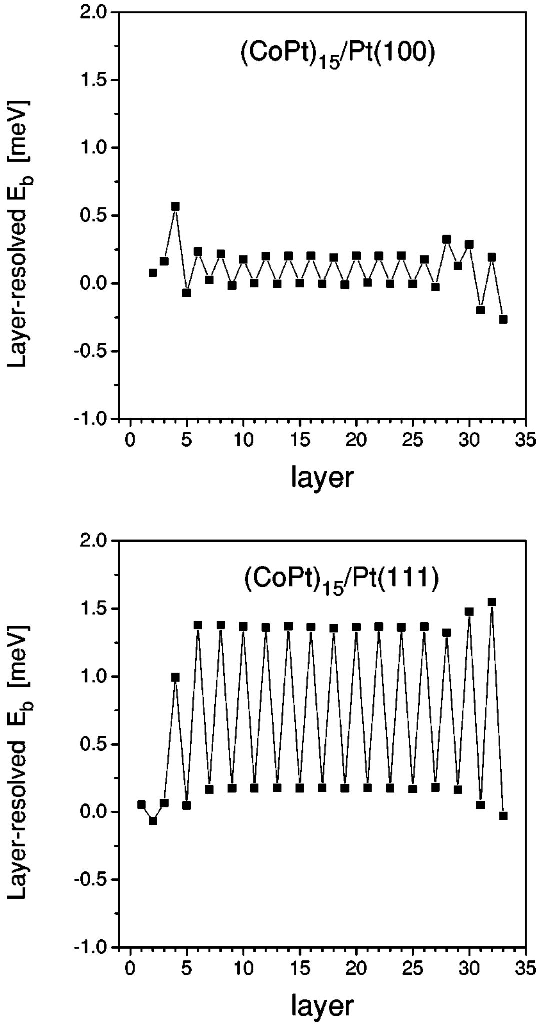

FIG. 6. Layer-resolved band energies for $(\mathrm{CoPt})_{15}/\mathrm{Pt}(100)$ (top) and $(\mathrm{CoPt})_{15}/\mathrm{Pt}(111)$ (bottom).

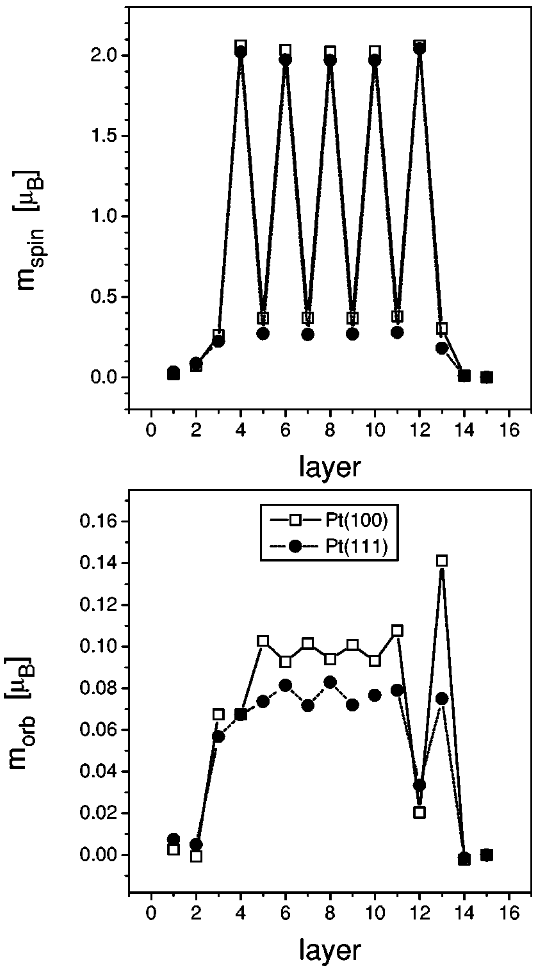

FIG. 7. Layer-resolved spin-only (top) and orbital (bottom) magnetic moments of $(\mathrm{CoPt})_5$ on Pt(100) (squares) and Pt(111) (circles).

namely, about $(0.2–0.3)\mu_B$. It is fairly obvious from Fig. 7 that, contrary to common usage, the orbital magnetic moments offer no explanation whatsoever for magnetic anisotropy phenomena. Quite clearly it is mostly the different geometrical arrangement that, in terms of the magnetic anisotropy energy, singles out the (111) orientation as compared to the (100) surface.

In Fig. 8 the spin-only moments of Co and Pt in $(\mathrm{Co}_{0.5}\mathrm{Pt}_{0.5})_n/\mathrm{Pt}(100)$ are displayed for $n \leqslant 10$. This figure shows, in particular, the importance of a sufficiently thick buffer for magnetic multilayers on a ‘‘nearly magnetic’’ metal. Worded differently, this figure shows the effect of the ‘‘polarization’’ of the top Pt substrate layers (the buffer) by the magnetic top: the magnetic moments in the buffer vary smoothly from zero (bulk value) over three layers to the value characteristic in the alloy. The layer-resolved Co moments in $(\mathrm{Co}_{0.5}\mathrm{Pt}_{0.5})$ on Pt(100) are fairly independent of the number of repetitions, and vary only slightly in the vicinity of the interfaces. This variation is shown explicitly in Fig. 9 by comparing the Co moments of the free surfaces of $\mathrm{Co}_{10}$ and $(\mathrm{Co}_{0.5}\mathrm{Pt}_{0.5})_{10}$ on Pt(100). As one can see, in the alloy case the Co moments are slightly larger than for pure Co, and the perturbation due to the interfaces with the substrate and at the surface is of the order of about $0.3\mu_B$. It should be noted that in the alloy case (Figs. 8 and 9) the magnetic moments are *not* weighted by the concentration. The average magnetic moment in the $i$th layer,

$$\langle m_i \rangle = \sum_{\alpha=A,B} c_i^{\alpha} m_i^{\alpha}, \tag{5}$$

only enters the determination of the magnetic dipole-dipole contribution $E_{\mathrm{dd}}$ to the anisotropy energy.[11] This in turn is the reason why, in Fig. 3, $E_{\mathrm{dd}}$ has roughly only half of the value of the corresponding quantities in Fig. 1.

## IV. COMPARISON TO EXPERIMENT AND DISCUSSION

Having now presented the theoretical results, it is relatively easy to compare with and to comment on available experimental data. It became customary to use a phenomenological ansatz of the following form for the magnetic anisotropy:

$$K_{\mathrm{eff}} = 2K_s/t + K_v, \tag{6}$$

where $K_v$ represents the so-called volume anisotropy constant, $K_s$ the so-called surface or interface contribution, and $t$ the layer thickness (in monolayers) of the magnetic top. Lin *et al.*,[12] e.g., found that in three sets of thin Co films on Pt,

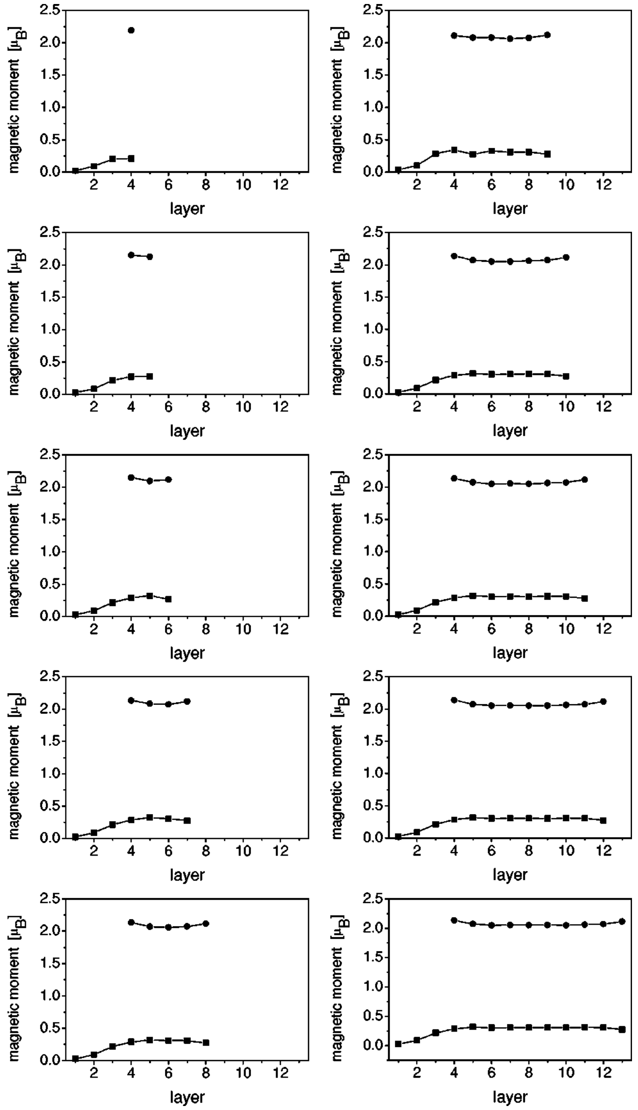

FIG. 8. Layer- and component-resolved spin-only magnetic moments of the free surface of $(\mathrm{Co}_{0.5}\mathrm{Pt}_{0.5})_n$ on Pt(100), $n \leqslant 10$. Circles refer to Co moments, squares to Pt moments.

$K_v$ is negative and seems to be independent of the crystallographic orientation of the surface. They also stated that the positive value of $K_s$ they found depends heavily on the orientation. These findings can be read off very nicely from Figs. 1, 4, and 5: there indeed is quite a difference in the contribution from the Co/Pt interface—the equivalent of $K_s$ being positive—with respect to different surface orientations, and—as already mentioned—$K_v$ is small and negative.

For $(\mathrm{Co}_r\mathrm{Pt}_s)_n$ superstructures on Pt(100), $r$ and $s$ being integers, the same authors[12] argued that there is a tendency toward a perpendicular anisotropy by decreasing $r$ to 1. Again it can be read off from Figs. 2 and 4 that indeed for the case $r = s = 1$, perpendicular magnetism has to be expected. Even more convincing is a comparison with a (CoPt)/Pt(111) superstructure, as Lin *et al.*[12] stated that such a system has a large perpendicular anisotropy, which is exactly what Figs. 2 and 4 show. Also, their observation that the orientational dependence of $K_{\mathrm{eff}}$ in the case of superstructures has to be correlated to the ''interfacial magnetic anisotropy'' and to ''polarized Pt atoms at the interface'' can be visualized directly from Fig. 6, showing the layerwise contributions to $E_b$, and from the spin-only moments in Fig. 7, from which the actual value of the Pt moments can be read off.

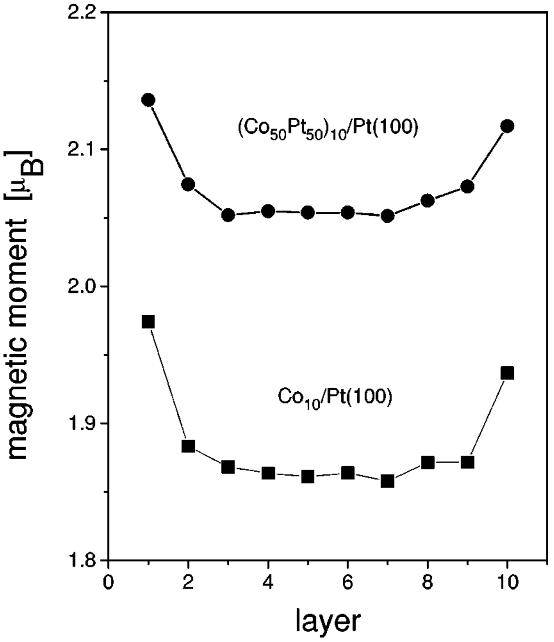

FIG. 9. Comparison between the Co-like moments for free surfaces of $(\mathrm{Co}_{0.5}\mathrm{Pt}_{0.5})_{10}$ (circles) and $\mathrm{Co}_{10}$ (squares) on Pt(100).

As compared to the study of McGee *et al.*[13] on ultrathin Co films on Pt(111), at a first glance the present results seem to disagree with their data, as up to a thickness of nine Co layers these authors found a perpendicular orientation of the magnetization with a particularly high value for $K_s$. However, as they did not measure free surfaces of Co on Pt(111), but had a Pt cap about 20 Å thick, only an indirect comparison can be made. From the middle row in Fig. 5 it is obvious that the main contributions to $E_b$ arise from the interfaces, the interface to vacuum being different than the one to Pt. Quite obviously, a second Co/Pt interface increases $E_b$, but it also doubles the possibility of interdiffusion at the interfaces, which in turn reduces the positive contribution from the interfaces to $E_b$, or, if ordering occurs, yields just the opposite.

From magnetic circular x-ray dichroism of Co on Pt(111) Thiele *et al.*[14] concluded that a minimum thickness of about 1.8 ML of Co is needed for a remanent magnetic ordering at room temperature, and claimed a critical thickness of about 7 ML of Co for the observation of a perpendicular magnetic anisotropy. However, they also argued that introducing a second Pt/Co interface by capping the system with Pt increases this critical thickness. Accepting their careful language with respect to selection rules in stating that their results seemed to indicate an enhancement of the Co orbital moment, it is worthwhile to mention that in the present calculations the Co orbital moment in the interior of a Co film on Pt(111) indeed is quite large, about $(0.14–0.15)\mu_B$.

From a previous study by this group[15] using Auger electron spectroscopy, it follows that annealing the films above about 250 °C leads to interdiffusion at the interfaces, and consequently to surface alloying and subsequent ordering effects. In a study of polycrystalline $\mathrm{Co}_c\mathrm{Pt}_{1-c}$, $c \approx 0.3$, Tyson *et al.*[16] claimed that they found the first evidence of phase separation in these films, leading to extended two-dimensional Co clusters in the film plane and to internal interfaces. Taking their experimental evidence, namely, that their perpendicular magnetic anisotropy is much smaller than those for an ordered superstructure, an interpretation of their data in terms of the present results can tentatively be given. Since in reasonably thick films of pure Co and statistically disordered $\mathrm{Co}_c\mathrm{Pt}_{1-c}$, $c=0.5$, on Pt(100) the magnetization is in-plane (see in particular Fig. 4), while for a superstructure of (CoPt) on the same substrate a perpendicular orientation has to be expected (see in particular Fig. 4), indeed the most likely explanation for their finding is the partial ordering in the samples investigated.

For very thick $\mathrm{CoPt}_3$ alloys (a film thickness of typically 3000 Å), it was found by Rooney *et al.*[17] that both the (111) and (100) orientations show a maximum of a perpendicular magnetic anisotropy around 400 °C. Although such systems cannot be compared directly to the present calculations, since they refer to a substrate of $\mathrm{CoPt}_3$ composition rather than Pt, it is interesting to remark that these authors suggested phase separation as an explanation of perpendicular magnetism, as indicated by Figs. 1–3. For bulk $\mathrm{CoPt}_3$ samples, resonant surface magnetic x-ray diffraction[18] suggests Pt surface segregation, which again induces strong compositional variations resulting in interesting kinds of ordering phenomena[19] that in turn can influence magnetic properties substantially.

Surface alloying with a Co-enriched top layer, for example, was traced by Ferrer *et al.*[20] when trying to grow thin films of Co on Pt(111). From their resonant magnetic surface diffraction measurements, they found that, as compared to bulk CoPt alloys in which the magnetic moments of Pt range from about $0.25\mu_B$ to $0.45\mu_B$, depending on the degree of order of the alloy and its composition, the topmost Pt layer next to Co in the Co/Pt interface is about $0.2\mu_B$, while the one from the second neighboring Pt layer carries only a moment of about $0.02\mu_B$. This estimate fits rather well to the results for the alloy case shown in Fig. 8, where the Pt moments in the buffer are in turn $0.027\mu_B$, $0.091\mu_B$, and $0.215\mu_B$, the last one referring to the Pt layer neighboring the first alloy layer.

## V. CONCLUSION

In conclusion, we can summarize that in the present paper the magnetic anisotropy properties of thin Co and of ordered and disordered (CoPt) alloy films on Pt(100) and Pt(111) were discussed in quite some detail. As the theoretical results are based on a relativistic, spin-polarized approach, no additional approximations such as a perturbative treatment of spin-orbit coupling are needed. The above discussion of experimental results shows very drastically that in comparing theoretical results with experimental data one has to be extremely careful. This applies in particular to magnetic anisotropy measurements, as not only a lattice constant mismatch but also interdiffusion and subsequent ordering quite likely control the occurrence of perpendicular magnetism. Once magnetic anisotropy effects are as robust as in the case of (ordered) superstructures, such as, e.g., on Pt(111), alloying effects are perhaps of less importance, or so it seems at the moment. It should be noted that for very well-characterized systems, results using the present approach yield almost perfect agreement with experimental determined magnetic anisotropy constants.[21] Therefore, if theoretical results like the present one disagree with experimental data in one aspect or the other, then obviously there is a good physical reason for such a discrepancy: interdiffusion, segregation, ordering, structural distortions, etc. Exactly these kinds of effects have to be sorted out in order to improve materials with perpendicular magnetic anisotropies.

## ACKNOWLEDGMENTS

This paper resulted from a collaboration partially funded by the TMR network on ‘‘*Ab initio* calculations of magnetic properties of surfaces, interfaces, and multilayers’’ (Contract No. EMRX-CT96-0089). Financial support was also provided by the Center of Computational Materials Science (Contract No. GZ 308.941), the Austrian Science Foundation (Contract Nos. P11626 and P12352), and the Hungarian National Science Foundation (Contract Nos. OTKA T024137 and T030240). We also wish to thank the computing center IDRIS at Orsay, as part of the calculations were performed on their Cray T3E machine.

---

[1] D. Weller, in *Spin-Orbit-Influenced Spectroscopies of Magnetic Solids*, edited by H. Ebert and G. Schütz (Springer-Verlag, Heidelberg, 1996), p. 1.

[2] S. S. A. Razee, J. B. Staunton, and F. J. Pinski, Phys. Rev. B **56**, 8082 (1997).

[3] J. M. McLaren and R. H. Victora, Appl. Phys. Lett. **66**, 3377 (1995).

[4] U. Nowak, J. Heimel, T. Kleinefeld, and D. Weller, Phys. Rev. B **56**, 8143 (1997).

[5] L. Szunyogh, B. Újfalussy, and P. Weinberger, Phys. Rev. B **51**, 9552 (1995).

[6] R. Zeller, P. H. Dederichs, B. Újfalussy, L. Szunyogh, and P. Weinberger, Phys. Rev. B **52**, 8807 (1995).

[7] L. Szunyogh, B. Újfalussy, P. Weinberger, and J. Kollár, Phys. Rev. B **49**, 2721 (1994).

[8] P. Weinberger, Philos. Mag. B **77**, 509 (1997).

[9] S. H. Vosko, L. Wilk, and M. Nusair, Can. J. Phys. **58**, 1200 (1980).

[10] P. Weinberger, P. M. Levy, J. Banhart, L. Szunyogh, and B. Újfalussy, J. Phys.: Condens. Matter **8**, 7677 (1996).

[11] J. Zabloudil, L. Szunyogh, U. Pustogowa, C. Uiberacker, and P. Weinberger, Phys. Rev. B **58**, 6316 (1998).

[12] C.-J. Lin, G. L. Gorman, C. H. Lee, R. F. C. Farrow, E. E. Marinero, H. V. Do, H. Notarys, and C. J. Chien, J. Magn. Magn. Mater. **93**, 194 (1991).

[13] N. W. E. McGee, M. T. Johnson, J. J. de Vries, and J. van de Stegge, J. Appl. Phys. **73**, 3418 (1993).

[14] J. Thiele, C. Boeglin, K. Hricovini, and F. Chevrier, Phys. Rev. B **53**, R11 934 (1996).

[15] J. Thiele, N. T. Barrett, R. Belkou, C. Guillot, and H. Kunodi, J. Phys.: Condens. Matter **6**, 5025 (1994).

[16] T. A. Tyson, S. D. Conradson, R. F. C. Farrow, and B. A. Jones,

Phys. Rev. B **54**, R3702 (1996).

[17] P. W. Rooney, A. L. Shapiro, M. Q. Tran, and F. Hellman, Phys. Rev. Lett. **75**, 1843 (1995).

[18] S. Ferrer, P. Fajardo, F. de Bergevin, J. Alvarez, X. Torrelles, H. A. van der Vegt, and V. H. Etgens, Phys. Rev. Lett. **77**, 747 (1996).

[19] G. R. Harp, D. Weller, T. A. Rabedeau, R. F. C. Farrow, and M. F. Toney, Phys. Rev. Lett. **71**, 2493 (1993).

[20] S. Ferrer, J. Alvarez, E. Lundgren, X. Torrelles, P. Fajardo, and F. Boscherini, Phys. Rev. B **56**, 9848 (1997).

[21] C. Uiberacker, J. Zabloudil, P. Weinberger, L. Szunyogh, and C. Sommers, Phys. Rev. Lett. **82**, 1289 (1999).