PHYSICAL REVIEW B **67**, 024415 (2003)

Magnetic properties of finite Co chains on Pt(111)

B. Lazarovits,[1] L. Szunyogh,[1,2] and P. Weinberger[1]
[1]*Center for Computational Materials Science, Technical University Vienna, A-1060, Gumpendorferstr. 1.a., Vienna, Austria*
[2]*Department of Theoretical Physics, Budapest University of Technology and Economics, Budafoki út 8, H-1521 Budapest, Hungary*

(Received 27 September 2002; published 21 January 2003)

We present *first-principles* calculations of the magnetic moments and magnetic anisotropy energies of finite monoatomic Co_n $(1 \leqslant n \leqslant 10)$ chains deposited along the (110) direction on top of a fcc Pt(111) surface. The calculations were performed fully relativistically using the embedded-cluster technique within the Korringa-Kohn-Rostoker method. The magnetic anisotropy energy was evaluated by means of the magnetic force theorem. As a direct consequence of the reduced coordination number of the Co atoms, we found enhanced spin and orbital moments as well as enhanced anisotropy energies in the Co chains as compared to a Co overlayer on Pt(111). For the Pt atoms adjacent to the Co atoms, however, we obtained induced magnetic moments smaller than in the case of a Co monolayer on Pt(111). The moments and the contributions of the individual atoms to the magnetic anisotropy energy depend characteristically on the position within the chains, i.e., on the local environment of the individual atoms. Independent of the length of the chains we found that the easy axis is perpendicular to the surface. The size of the calculated magnetic anisotropy energy and of the anisotropy of the orbital moment fits very well to available experimental values for monoatomic Co chains deposited on a Pt(997) surface.

DOI: 10.1103/PhysRevB.67.024415 PACS number(s): 75.30.Hx, 73.22.−f, 71.70.Gm, 75.30.Gw

I. INTRODUCTION

The electronic and in particular the magnetic properties such as magnetic moments and the magnetic anisotropy energy (MAE) of transition metals are very sensitive to the local environment and the dimensionality of the system. Due to advanced manufacturing techniques well characterized low-dimensional structures are nowadays available and intensively studied.[1–18] Experiments on Fe nanostripes on a W(110) surface[1,4] called the attention to the unique features of such systems. For Fe stripes on Cu(111) Shen *et al.*[3] observed an easy axis perpendicular to the surface and found that the magnetization was temperature and time dependent. Recently, York *et al.*[5] demonstrated that at definite growth conditions, Co can form self-organized arrays of nanowires on a Cu(110) surface. Monoatomic rows of Ag, Cu, and Co can be grown on a periodically stepped surface of Pt as decoration.[6,7] Co wires on Pt exhibit exorbitant magnetic properties like unusually large orbital moments and strong magnetic anisotropies if compared to a monolayer or the bulk case.[8] In these experiments the estimated average length of a continuous Co chain was 80 atoms; at a temperature of 45 K the ferromagnetic order was, however, found to extend over about 15 Co atoms only.

Concomitantly with these experiments, quite some theoretical effort was devoted to study magnetism in one-dimensional (1D) arrangements of atoms deposited on surfaces. Effects of interatomic electronic interactions on the formation of magnetic moments were discussed in details for finite[9] and infinite[14] $4d$ atomic chains on flat and vicinal Ag surfaces, leaving however, questions about the oscillatory behavior of the moments open. The structure and magnetism of monoatomic Fe wires grown on different stepped Cu(11n) $(n=3-11)$ surfaces were investigated by Spišák and Hafner.[15] The magnetic anisotropy energy (MAE) of one-dimensional transition-metal nanostructures has also been calculated in terms of tight-binding techniques.[11,12] In particular, Dorantes-Dávila and Pastor[12] revealed that oscillations of the MAE corresponding to a preferred orientation along short Fe and Co wires are stabilized over a length of about 20 atoms. They found that when deposited on Pd(110) the magnetization of the Co wires turned to an out-of-plane direction. Eisenbach *et al.*[16] demonstrated that changing the crystallographic orientation of infinite Fe wires embedded into Cu bulk can even result in a change of the easy axis. Very recently Komelj *et al.*[17] established a clear trend for an enhancement of the spin and orbital magnetism of Co as bulk (3D), monolayer (2D), and wire (1D), respectively.

In the present paper we study the magnetic properties of Co_n chains of different length $(1 \leqslant n \leqslant 10)$ deposited along the (110) direction of a Pt(111) surface in terms of *ab initio* calculations. Focusing on the spin and orbital moments as well as on the MAE we trace in particular the crossover between a pointlike impurity (0D) and a linear chain (1D). We also compare our results to the values measured for monoatomic Co chains grown at the step edges of Pt(997).[8]

II. THEORETICAL APPROACH

Self-consistent fully relativistic calculations for finite Co chains along the (110) direction on Pt(111) have been performed by using the embedded-cluster technique within multiple-scattering theory in which the matrix of the so-called scattering path operator (SPO) $\boldsymbol{\tau}_{\mathcal{C}}$ corresponding to a cluster $\mathcal{C}$ can be obtained from the following Dyson equation:[19]

$$\boldsymbol{\tau}_{\mathcal{C}}(E)=\boldsymbol{\tau}_h(E)\{\boldsymbol{I}-[\boldsymbol{t}_h^{-1}(E)-\boldsymbol{t}_{\mathcal{C}}^{-1}(E)]\boldsymbol{\tau}_h(E)\}^{-1}, \qquad (1)$$

where $\boldsymbol{t}_h(E)$ and $\boldsymbol{\tau}_h(E)$ denote the single-site scattering and the SPO matrix for the unperturbed host sites in cluster $\mathcal{C}$, respectively, while $\boldsymbol{t}_{\mathcal{C}}$ refers to the single-site scattering matrices of the perturbing atoms. Note that Eq. (1) takes into account all scattering events both inside and outside the cluster. Once $\boldsymbol{\tau}_C$ is calculated, one can in turn calculate all quantities of interest, i.e., charge and magnetization densities, spin and orbital moments, etc.[19]

The self-consistent calculations of the host Pt(111) surface were performed in terms of the fully relativistic screened Korringa-Kohn-Rostoker method,[20,21] using layers of empty sites to represent the vacuum region. The magnetic adatoms occupied sites in the first vacuum layer. No attempts were made to include lattice relaxation effects: the host and the cluster sites refer therefore to the positions of an ideal fcc parent lattice with the experimental Pt lattice constant (3.92 Å). The local spin-density approximation as parametrized by Vosko *et al.*[22] was applied, the effective potentials and fields were treated within the atomic sphere approximation (ASA). When solving the Kohn-Sham-Dirac equation and also for the multipole expansion of the charge densities, necessary to evaluate the Madelung potentials, a cutoff of $\ell_{max}=2$ was used.

By using the self-consistent potentials with a magnetization orientation pointing perpendicular to the surface (along the z axis), we calculated the MAE by means of the magnetic force theorem[23,24] as differences of band energies,[19]

$$\Delta E_{x-z}=E_x^b-E_z^b \quad \text{and} \quad \Delta E_{y-z}=E_y^b-E_z^b, \tag{2}$$

$$\Delta E_{\mu-z}=\begin{cases} >0, & z \text{ preferred} \\ <0, & \mu \text{ preferred} \end{cases}; \quad \mu=x,y, \tag{3}$$

where the axes x and y refer to in-plane directions parallel and perpendicular to the chains, respectively. Applying this formalism, the MAE can be resolved into contributions with respect to atoms. It should be noted that in this paper we neglected the magnetic dipole-dipole interaction part of the MAE.[23]

III. SPIN AND ORBITAL MOMENTS

Because of the spatially extended $5d$ states of Pt, a relatively strong interaction between electronic states corresponding to the Co and the Pt atoms is to be expected. For the case of a single Co adatom therefore we carefully investigated the sensitivity of the local physical properties of the Co adatom with respect to the size of the environment by incorporating self-consistently treated Pt substrate atoms. We performed calculations up to the fourth neighboring shell of Pt atoms around the Co adatom and found that in treating only the first shell of neighbors self-consistently results in to a relative deviation of less than 1% of the local charge and the moments of Co as compared to the case when all the four neighboring shells were treated self-consistently. Therefore, if not stated otherwise, in the following all calculations refer to clusters containing only Pt atoms adjacent to the Co atoms.

Figure 1 shows the spin (S_z) and orbital (L_z) moment of the central (most symmetric) atom of the monoatomic Co$_n$ wires ($1\leqslant n\leqslant 10$). First of all we notice that the spin moment of a single adatom ($2.21\mu_B$) is by about 10% larger than in the corresponding monolayer case ($2.00\mu_B$). This spin moment decreases with an increasing number of atoms forming the chain: in the case of a dimer we found $S_z=2.17\mu_B$ while for the central atom of a trimer $S_z=2.12\mu_B$. The reason of this trend can clearly be traced from Fig. 2, where the spin-projected densities of states (DOS) (Refs. 21 and 25) of the corresponding Co atoms are displayed: for a Co adatom, the Fermi level crosses the very sharp peak of the minority spin d band, which, as a consequence of the d-d hybridization between the Co atoms, remarkably broadens in the dimer and trimer case thus pushing more states below the Fermi level than above. For $n>3$ the spin moment of the central atom seems to be stabilized at about $2.11\mu_B$, which despite the different geometry is in good comparison to the experimental value of about $2.12\mu_B$,[8] and other LDA (FLAPW) calculations [$2.06\mu_B$ (Ref. 17)], for monoatomic Co chains on Pt(997).

The spin moments calculated for each of the Co atoms in

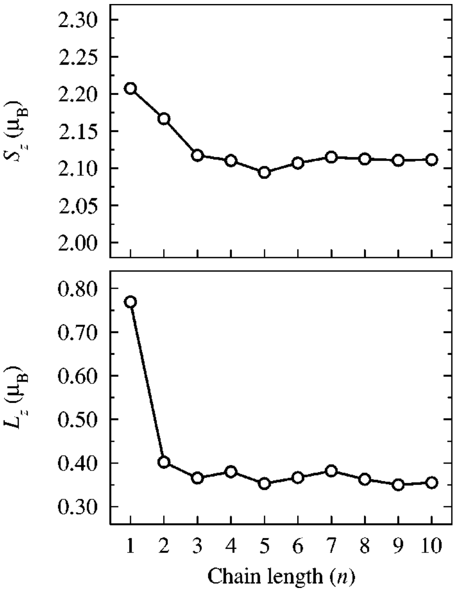

FIG. 1. Calculated spin moments (S_z) and orbital moments (L_z) of the central (most symmetric) atom in Co$_n$ ($n=1,\ldots,10$) chains oriented along the (110) direction on the top of Pt(111) as a function of the chain length.

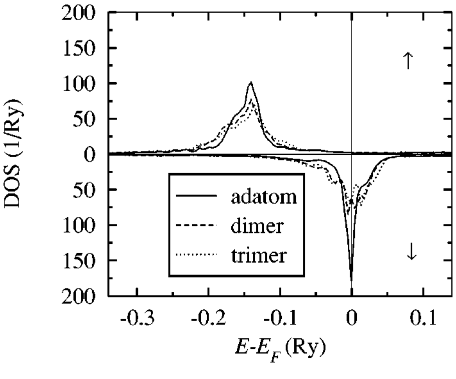

FIG. 2. Spin-projected local densities of states (DOS) of Co as an adatom, a dimer atom, and the central atom of a trimer on top of a Pt(111) surface.

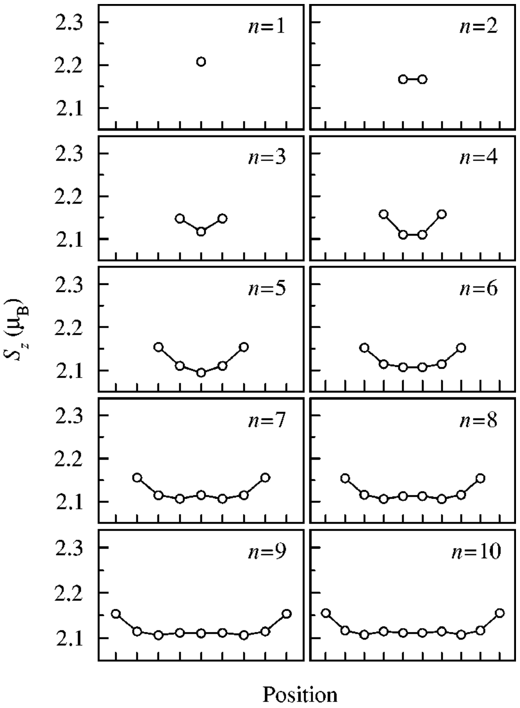

FIG. 3. Calculated spin moments (S_z) of the Co atoms in Co$_n$ ($n=1,\ldots,10$) chains on Pt(111) with the magnetization pointing perpendicular to the surface.

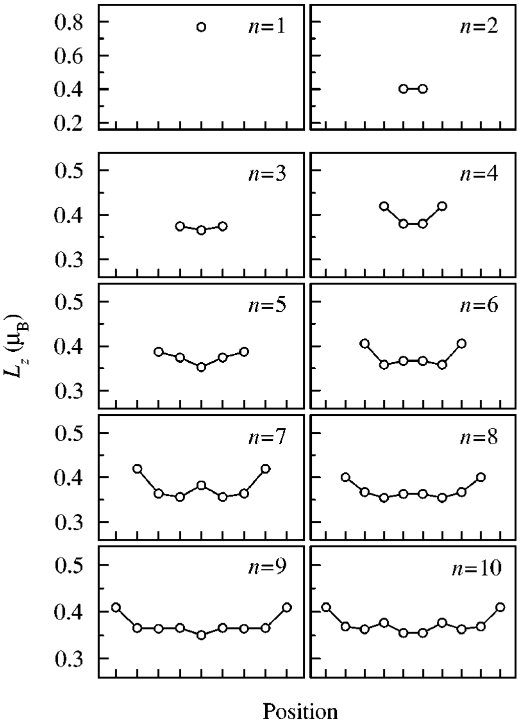

FIG. 4. Calculated orbital moments (L_z) of the Co atoms in Co$_n$ ($n=1,\ldots,10$) chains on Pt(111) with the magnetization pointing perpendicular to the surface.

the chains are shown in Fig. 3. Apparently, for $n=3,\ldots,10$, the spin moments at the end of the chains ($\sim 2.15\mu_B$) are systematically higher than those in the middle of the chains ($\sim 2.11\mu_B$). This observation can again be attributed to the narrower minority spin d band of the outer atoms due to one missing neighboring Co atom as compared to the inner atoms (see also Fig. 2). It should be noted, however, that the above feature cannot be stated as a general feature, since the relation of the spin moments of the outer and inner atoms in a linear chain can vary according to the varying nature of the d-d hybridization between transition-metal atoms.[9] Contrary to the magnetic moments of compact $3d$ clusters which tend rapidly to the monolayer value,[19] independent of their length the wires are characterized by larger magnetic moments than the corresponding monolayer. This is one of the unique features of the nanowires which distinguishes them from other types of nanoclusters.

Inspecting the orbital moments from the lower panel of Fig. 1, the case of a single adatom distinctly differs from all other cases, since the huge orbital moment of the Co adatom, $0.77\mu_B$, immediately decreases to $0.40\mu_B$ in the dimer and remains in the range of 0.35-0.40μ_B for the central atom of all longer chains. This implies that the orbital moments of the Co atoms are more sensitive to the chemical environment than the corresponding spin moments. Since the value for a Co monolayer on Pt(111) amounts only to $0.15\mu_B$, from the above results a clear trend of the Co orbital moment with respect to the dimensionality of the system (0D, 1D, 2D) can be read off.

Figure 4 shows that the fluctuations of the orbital moments within the chains are somewhat larger than for the spin moments (compare to Fig. 3). As can be seen, the orbital moments of the central and the outer atoms can even differ by more than 10% and also the variations at inner sites are remarkable. Nonetheless, similar to the spin moments (see Fig. 3) for the inner atoms of the longer chains a tendency of forming a uniform orbital magnetization can be observed. Based on Fig. 1, we numerically fitted the Co orbital moment of the central atom to the case of an infinite chain. The thus obtained value of $0.36\mu_B$ is smaller than the experimental value, $0.68\pm0.05\mu_B$.[8] For the step-edge-like geometry used in Ref. 17 an even smaller orbital moment ($0.16\mu_B$) was obtained, while using an orbital polarization scheme[26] resulted in a value of $0.92\mu_B$. While spin-polarized relativistic calculations usually underestimate the orbital part of the magnetization, in systems with reduced dimension the orbital polarization scheme seems to overestimate the orbital moments and, more peculiar, the size of the MAE.[27,28]

It is indeed worthwhile to discuss the spin and orbital polarization of the Pt atoms close to Co sites. Depending on the position with respect to the Co chain we found induced Pt spin moments of 0.09–0.14μ_B and orbital moments in the range of 0.02–0.04μ_B. These values are typically half as large as the corresponding moments considering a Pt(111) surface covered by a Co monolayer ($0.22\mu_B$ and $0.05\mu_B$, respectively). This decrease of the magnetic moments of Pt is apparently caused by the reduced number of the neighboring magnetic (Co) atoms, the actual source of the induced spin polarization at the Pt sites. This observation agrees well with other theoretical results for a Co chain placed on Pd (Ref. 13 and $3d$ impurities on Pd(001) and Pt(001) surfaces.[10] In

TABLE I. Calculated moments (in units of μ_B) of Pt atoms in a cluster with one Co impurity on top of a Pt(111) surface. N_i: number of sites in the ith shell of neighboring Pt atoms; S_z^i and L_z^i: average spin and orbital moments in shell no. i, S_z, and L_z: total sum of spin and orbital moments of Pt atoms up to shell (i).

i	N_i	S_z^i	L_z^i	S_z	L_z
1	3	0.093	0.024	0.279	0.071
2	12	0.013	0.002	0.439	0.093
3	3	<0.001	-0.001	0.441	0.089
4	16	0.003	0.001	0.493	0.107

Table I the induced spin and orbital moments of Pt are shown treating four shells of Pt atoms self-consistently in the neighborhood of a Co impurity on top of a Pt(111) surface. Although the induced moments in the individual shells rapidly decrease with increasing distance from the Co impurity, the increasing number of Pt atoms gives rise to a slowly convergent total sum of moments. In particular, due to the Pt atoms, for longer chains an enhancement of the orbital moment of about $0.1\mu_B$ per Co atom can be estimated, which clearly improves the agreement between our calculations and the experiment (see above).

IV. MAGNETIC ANISOTROPY

The induced moments on the Pt sites also imply that a considerable contribution to the MAE arises from the Pt atoms around the Co chains. Therefore in the case of a single Co adatom we again investigated the effect of the first four nearest-neighboring Pt shells on the MAE. We found that the contributions from the Pt atoms decrease rapidly with increasing distance from the Co atom and that the difference in the total MAE is less than 7% between the case when only the first shell and when all four shells of Pt atoms are included into the calculations. In the case of longer chains the Pt atoms in the first-nearest shell contribute to the MAE in a similar manner (0.2–0.4 meV/atom depending on the position) as in the case of the adatom. Thus, also for the calculation of the MAE we only considered the first Pt shell around the Co atoms with an estimated relative error of less than 10% which seems to be a good compromise between the accuracy of the calculations and the numerical efforts required.

In Fig. 5 the magnetic anisotropy energies ΔE_{x-z} and ΔE_{y-z} including only contributions from the first shell of Pt sites (see above) and normalized to a single Co atom are shown with respect to the length of the Co chains. As can be seen from the positive sign of the MAE, in each case the easy axis points perpendicular to the surface, whereby for $n \geqslant 2$ there also appears a strong in-plane anisotropy with a preference of the x direction, i.e., parallel to the chains. It is interesting to mention that as compared to a single adatom we found in the case of small $(1 \leqslant n \leqslant 3)$ linear clusters of Co on Ag(100) a reorientation of the easy axis from out-of plane to an in-line direction for the dimer and trimer.[19] The huge MAE of a single Co adatom, $\Delta E_{x-z} = \Delta E_{y-z} = 5.9$ meV, abruptly drops for the dimer and rapidly converges to $\Delta E_{x-z} \simeq 1.5$ meV and $\Delta E_{y-z} \simeq 3.3$ meV for the longer wires. Evidently, the experimental easy axis of the Co/Pt(997) chains, perpendicular to the chains and 43° away from the normal of the (111) planes,[8] could not be confirmed by our calculations. Nevertheless, the fact that the calculated easy axis points out-of-plane and is perpendicular to the chains, and also that the size of our calculated MAE is very close to the measured value of 2 ± 0.2 meV, can still be termed a nice agreement between experiment and theory.

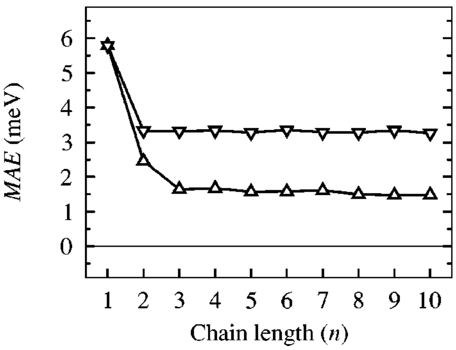

FIG. 5. Calculated magnetic anisotropy energies (MAE) for Co_n $(n=1,\ldots,10)$ chains on Pt(111) including also contributions from nearest-neighbor Pt sites and normalized to one Co atom. Up and down triangles refer to ΔE_{x-z} and ΔE_{y-z}, respectively [see Eq. (2)].

The contributions of the individual Co atoms, $\Delta E_{x-z}^{\mathrm{Co}_i}$ and $\Delta E_{y-z}^{\mathrm{Co}_i}$ $(i=1,\ldots,n)$, to the MAE are displayed in Fig. 6. In case of $(x-z)$, the largest contributions clearly come from the outer Co atoms, while in the $(y-z)$ case the contribution of the inner atoms to the MAE is nearly as big as the contribution of outer atoms. In both cases considered namely ΔE_{x-z} and ΔE_{y-z}, only weak oscillations in the MAE can be seen for the longer chains.

The anisotropies of the orbital moments are shown in Fig. 7. In the case of a single adatom the anisotropy of the orbital moment $\Delta L_{x(y)-z} = L_{x(y)} - L_z = -0.27\mu_B$ obeys the qualitative rule that the orbital moment is largest along the easy axis.[29] As can be seen from Fig. 7, this rule applies also to the chains since along the y direction (hard axis) the orbital moments of all the Co atoms are by about $0.15\mu_B$ less than along the z direction (easy axis) $(\Delta L_{y-z} = -0.15\mu_B)$. Note that this value is close to that given experimentally, namely, $0.12\mu_B$.[8] The anisotropy of the orbital moments of the Co atoms with respect to the x and z directions (ΔL_{x-z}), however, is only a few of $0.01\mu_B$, and in several cases changes even sign from site to site. This situation is quite unusual since the tiny orbital momentum anisotropies are to be compared with quite sizeable respective magnetic anisotropy energies, $\Delta E_{x-z}^{\mathrm{Co}_i} \simeq 0.5$–1.5 meV. In terms of perturbation theory this implies that for the $(x-z)$ case, significant spin-flip coupling induced by the spin-orbit interaction may contribute to the MAE which, in turn, obscures the simple (inverse) proportionality between the MAE and the anisotropy of the orbital moment.[30]

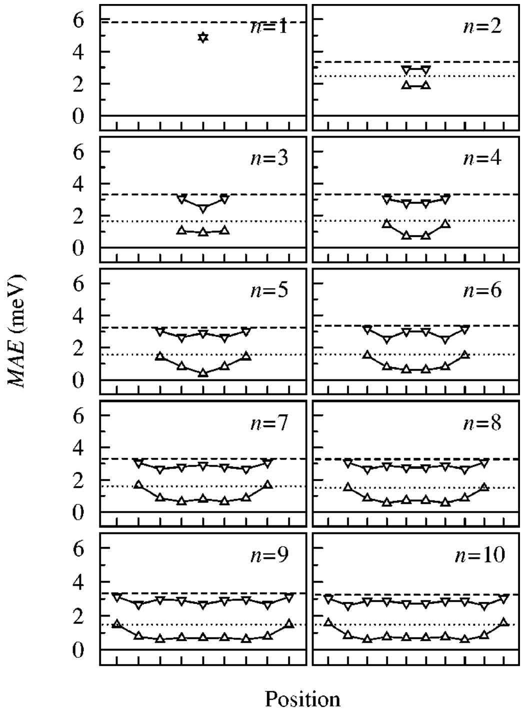

FIG. 6. Contributions of the individual Co sites to the MAE of Co$_n$ ($n=1,\ldots,10$) chains on Pt(111). Up and down triangles refer to $\Delta E^{\mathrm{Co}_i}_{x-z}$ and $\Delta E^{\mathrm{Co}_i}_{y-z}$ ($i=1,\ldots,n$), respectively. For comparison, the corresponding MAE of the chains normalized to one Co atom is marked by dots (ΔE_{x-z}) and dashes (ΔE_{y-z}).

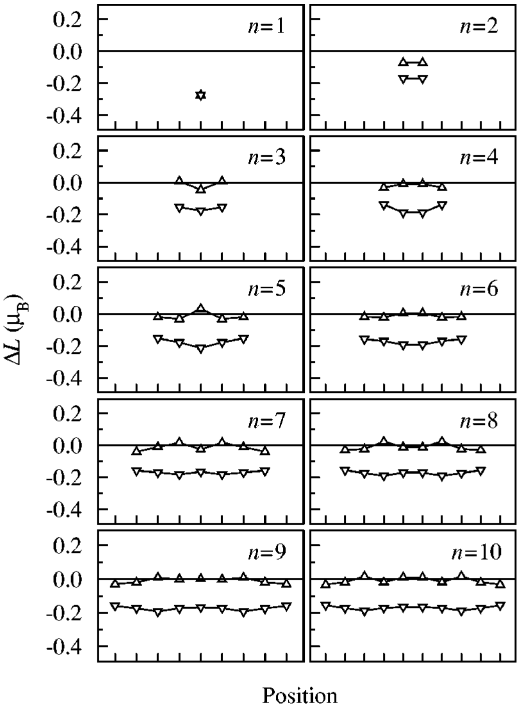

FIG. 7. Anisotropy of the orbital moments of the Co sites in Co$_n$ ($n=1,\ldots,10$) chains on Pt(111). Up and down triangles refer to ΔL_{x-z} and ΔL_{y-z}, respectively.

V. CONCLUSIONS

Employing a real-space embedded-cluster technique based on the Korringa-Kohn-Rostoker Green's-function method, we have carried out fully relativistic self-consistent calculations for finite Co chains oriented along the (110) direction on top of a Pt(111) surface. As compared to the overlayer (2D) case, Co|Pt(111), due to the decreased coordination number we obtained largely enhanced spin and orbital moments as well as magnetic anisotropy energies, which are systematically smaller than those obtained for a single adatom (0D). For all the quantities under consideration we found fast convergence when increasing the length of the chains. Thus from the values of the central atom the corresponding quantities for the infinite chain (1D) could easily be estimated. These extrapolated results were then compared to the corresponding experimental values for long Co chains on Pt(997).[8] Although a different geometry was used in our calculations, the spin moment of the Co atoms, the easy axis of the system, the size of the MAE and also the anisotropy of the orbital moment is in good agreement with experiment.

We showed that as far as local quantities are concerned from calculations for rather short linear chains properties characteristic for long (ideally infinite) chains can be deduced without losing the possibility to study local fluctuations (finite-size effects) within the chains. Obviously, when investigating, e.g., (magneto)transport properties of such nanostructures, due to the nonlocality of the transport phenomena, a less evident trend with respect to the size of the nanoclusters has to be expected.

ACKNOWLEDGMENTS

This paper resulted from a collaboration partially funded by the RTN network ''Computational Magnetoelectronics'' (Contract No. RTN1-1999-00145). Financial support was also provided by the Center for Computational Materials Science (Contract No. GZ 45.451), the Austrian Science Foundation (Contract No. W004), and the Hungarian National Scientific Research Foundation (OTKA T030240 and OTKA T037856).

---

[1] H. J. Elmers, J. Hauschild, H. Houmlche, U. Gradmann, H. Bethge, D. Heuer, and U. Koumlhler, Phys. Rev. Lett. **73**, 898 (1994).

[2] M. F. Crommie, C. P. Lutz, D. M. Eigler, and E. J. Heller, Physica D **83**, 98 (1995).

[3] J. Shen, R. Skomski, M. Klaua, H. Jenniches, S. S. Manoharan, and J. Kirschner, Phys. Rev. B **56**, 2340 (1997).

[4] J. Hauschild, H. J. Elmers, and U. Gradmann, Phys. Rev. B **57**, R677 (1998).

[5] S. M. York and F. M. Leibsle, Phys. Rev. B **64**, 033411 (2001).

[6] P. Gambardella, M. Blanc, H. Brune, K. Kuhnke, and K. Kern, Phys. Rev. B **61**, 2254 (2000).

[7] P. Gambardella, M. Blanc, L. Bürgi, K. Kuhnke, and K. Kern, Surf. Sci. **449**, 93 (2000).

[8] P. Gambardella, A. Dallmeyer, K. Maiti, M. C. Malagoli, W. Eberhardt, K. Kern, and C. Carbone, Nature (London) **416**, 301 (2002).

[9] K. Wildberger, V. S. Stepanyuk, P. Lang, R. Zeller, and P. H. Dederichs, Phys. Rev. Lett. **75**, 509 (1995).

[10] V. S. Stepanyuk, W. Hergert, K. Wildberger, R. Zeller, and P. H. Dederichs, Phys. Rev. B **53**, 2121 (1996).

[11] R. Družinić and W. Hübner, Phys. Rev. B **55**, 347 (1997).

[12] J. Dorantes-Dávila and G. M. Pastor, Phys. Rev. Lett. **81**, 208 (1998).

[13] R. Robles, J. Izquierdo, and A. Vega, Phys. Rev. B **61**, 6848 (2000).

[14] V. Bellini, N. Papanikolaou, R. Zeller, and P. H. Dederichs, Phys. Rev. B **64**, 094403 (2001).

[15] D. Spišák and J. Hafner, Phys. Rev. B **65**, 235405 (2002).

[16] M. Eisenbach, B. L. Györffy, G. M. Stocks, and B. Újfalussy, Phys. Rev. B **65**, 144424 (2002).

[17] M. Komelj, C. Ederer, J. W. Davenport, and M. Faehnle, cond-mat/0207561 (unpublished).

[18] F. J. Himpsel, J. E. Ortega, G. J. Mankey, and R. F. Willis, Adv. Phys. **47**, 511 (1998).

[19] B. Lazarovits, L. Szunyogh, and P. Weinberger, Phys. Rev. B **65**, 104441 (2002).

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

[21] L. Szunyogh, B. Újfalussy, P. Weinberger, and J. Kollár, J. Phys.: Condens. Matter **6**, 3301 (1994).

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

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

[24] H. J. Jansen, Phys. Rev. B **59**, 4699 (1999).

[25] J. B. Staunton, B. L. Györffy, J. Poulter, and P. Strange, J. Phys. C **21**, 1595 (1988).

[26] M. S. Brooks, Physica B & C **130B**, 6 (1985).

[27] B. Lazarovits, diploma theses, Budapest University of Technology and Economics, 2000.

[28] B. Nonas, I. Cabria, R. Zeller, P. H. Dederichs, T. Huhne, and H. Ebert, Phys. Rev. Lett. **86**, 2146 (2001).

[29] G. van der Laan, J. Phys.: Condens. Matter **10**, 3239 (1998); P. Bruno, Phys. Rev. B **39**, 865 (1989).

[30] J. Stöhr, J. Magn. Magn. Mater. **200**, 470 (1999).