Magnetic behavior of monoatomic Co wires on Pd(110)

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The magnetic properties of monoatomic Co wires supported on the Pd(110) substrate have been studied using a self-consistent *spd*-tight-binding model with parameters fitted to *ab initio* tight-binding linear muffin-tin orbital results for the ideal Co monolayer deposited on the same substrate. The geometrical structure of the system is based on recent scanning tunneling microscopy experiments for Cu wires supported on Pd(110). Two possible magnetic configurations have been considered, one with parallel (P) magnetic coupling between adjacent wires and the other with antiparallel (AP) coupling. Results are reported for the local magnetic moments and spin-polarized densities of states, magnetic coupling between wires as a function of the interwire distance and wire-substrate magnetic interaction.

I. INTRODUCTION

The development of magnetic devices constitutes one of the most important tasks in high technology. The magnetic storage industry continues with plans of increasing growing rate in areal storage density. In addition, miniaturization represents another important field of development. These technologies require a consistent progress in many areas like giant magnetoresistance, spin valve read sensors, magnetic domain size reduction and others.

After the first experiments related with magnetoresistance in transition metal multilayers,[1,2] increasing attention has been focused on the possibility of building new samples consisting of supported nanostructures. This opens the possibility, as discussed before, of the development of extremely compact devices with new magnetic properties associated with the low-dimensional character of the supported structures. As in the case of the multilayers, the most interesting systems are those in which the substrate and the supported element have different magnetic behaviors and whose interface might play a particular role. Among the different supported nanostructures, the nanowires deserve particular attention because they combine the properties typical of supported clusters with those related with the confinement in one dimension. Several transport properties like the strong reduction of the scattering[3] or the quantization of the conductivity[4] have been found a few years ago in this class of materials. However, from the magnetic point of view these promising systems are rather new. In this context, most of the progress made so far is related with the experimental techniques of their production at different size scales.

Scanning tunneling microscopy (STM) manipulation at atomic scale[5] allows the formation of small atomic lines. Other techniques like decomposition of a metalorganic gas produced on the tip of a STM,[6] electrochemical deposition on a membrane[7] or focalized deposition with laser[8] produce long supported wires but with relatively large width (typically 600 Å). Very recently it has been shown the possibility of having a regular distribution of nanowires nucleated on the steps of vicinal surfaces.[9,10] However, the obtained wires have imperfections and widths which are far from the monoatomic. These studies show that it is possible to exploit the symmetry of the surface. This was the idea of Bucher and co-workers[10,11] for the growth of quasi-one-dimensional wires of a fcc transition metal on a (110) surface of an fcc substrate. In particular, these authors have obtained, at low temperatures ($T<300$ K), monoatomic wires of Cu with various hundreds Å length deposited on the Pd (110) substrate and oriented along the $(1\bar{1}0)$ direction.

Concerning the magnetic properties of transition-metal (TM) supported nanowires, several questions deserve to be investigated: magnetic order and magnetic coupling between wires as a function of interwire distance, average magnetic moment of the system, wire-substrate magnetic interaction, magnetic anisotropy. For technological purposes one would like to assemble atomic wires optimizing their packing, but this packing may have a limit because if the wires are too close together the intrinsic properties of the wires can be lost. In some natural alloys the identity of small clusters is maintained by the effect of some buffer atoms that act as a shield preventing the clusters from collapsing into larger entities.[12] The same effect has been applied in self-assembled artificial devices, where large metallic clusters are covered by a shield of organic molecules.[13] Knowing the characteristic length determining the interaction between wires is then of extreme importance for constructing efficient wire assemblies. The experimental characterization of the magnetic properties of TM supported nanowires is rather limited, particularly in which concerns the local magnetic behavior. At the same time, theoretical studies simulating the realistic samples experimentally accessible are extremely expensive due to the large number of inequivalent sites. In particular, *ab initio* methods based in a supercell are not computationally efficient in this context, being more adequate a model formulated in the real space that combines flexibility and a sufficient degree of accuracy.

As a first step in the understanding of the magnetic behavior of this new class of materials, we present a theoretical study of monoatomic Co wires supported on Pd(110). The Co/Pd interface have attracted the attention of the Scientific Community during the last decade. In particular, Co/Pd multilayers have been studied since 1985 due to their perpendicular anisotropy which makes them suitable for magneto-optic devices.[14] Perpendicular magnetic anisotropy has been

also predicted in a recent work[15] for a monoatomic Co wire supported on Pd(110). This opens the possibility of developing a new class of magneto-optic materials. The morphology of the system studied in the present work is modeled following the experimental results of Bucher and co-workers[10,11] for Cu wires on Pd(110). The same atomic arrangement is expected for Co deposited on the same substrate.[16] The spin-polarized electronic structure of the system is determined by self-consistently solving a semiempirical *spd*-band model Hamiltonian formulated in the real space and parametrized to *ab initio* tight-binding linear muffin-tin orbital (TB-LMTO) calculations for the ideal Co monolayer supported on Pd(110). In the next section we present this theoretical model and discuss the transferability of the parametrization. Results for the local magnetic moment, possible magnetic coupling between the Co wires as a function of the interwire distance, average magnetic moment, and possible induced spin polarization at Pd in the neighborhood of the Co wires are presented and discussed. The main conclusions of the present study are summarized at the end.

II. THEORETICAL MODEL

A. The Hamiltonian

The electronic structure is determined by solving self-consistently a tight-binding Hamiltonian for the $3d$, $4s$, $4p$ valence electrons in a mean-field approximation:

$$H=\sum_{i,\alpha,\sigma}\epsilon_{i\alpha\sigma}N_{i\alpha\sigma}+\sum_{\substack{i,\alpha,\sigma\\ i\neq j}}t_{ij}^{\alpha\beta}c_{i\alpha\sigma}^{\dagger}c_{j\beta\sigma}. \tag{1}$$

Here $c_{i\alpha\sigma}^{\dagger}$ ($c_{j\beta\sigma}$) are the operators for the creation (annihilation) of an electron with spin σ in the orbital state α (β) at the atomic site i (j), $N_{i\alpha\sigma}$ is the corresponding number operator. The electronic delocalization within the system is described by the hopping integrals $t_{ij}^{\alpha\beta}$ between orbitals α and β at sites i and j, which we consider up to second neighbors and are assumed to be spin independent. The hopping integrals between atoms of the same element are taken from a fit to reproduce the *ab initio* band-structure calculations for the pure element.[17] The heteronuclear hoppings at the Co-Pd interface are obtained as the average of the corresponding homonuclear hoppings.

The spin-dependent diagonal terms $\epsilon_{i\alpha\sigma}$ include the electron-electron interaction through a correction shift of the energy levels:

$$\epsilon_{i\alpha\sigma}=\epsilon_{i\alpha}^{0}+z_{\sigma}\sum_{\beta}\frac{J_{i,\alpha\beta}}{2}\mu_{i\beta}+\Omega_{i\alpha}. \tag{2}$$

$\epsilon_{i\alpha}^{0}$ are the bare energy of the orbital α at site i (that is, excluding Coulomb interactions). The second term is the correction shift due to the spin-polarization of the electrons at site i ($\mu_{i\beta}=\langle N_{i\beta\uparrow}\rangle-\langle N_{i\beta\downarrow}\rangle$). In this second term, $J_{i,\alpha\beta}$ are the exchange integrals and z_{σ} is the sign function ($z_{\uparrow}=+1$; $z_{\downarrow}=-1$). We neglect the exchange integrals involving sp electrons and the one corresponding to the d electrons is fitted to obtain the *ab initio* TB-LMTO value for the magnetic moment of the Co monolayer deposited on Pd(110) for the ferromagnetic-in-plane configuration. Finally, the site and orbital-dependent potentials $\Omega_{i\alpha}$ are self-consistently determined in order to obtain the *ab initio* sp- and d-electronic occupations of the Co monolayer on Pd(110). This is a good approximation due to the small charge transfer in TM systems.[18,20] The details of this fit as well as the transferability of the parametrization are discussed in the last subsection.

B. Self-consistent calculation

The magnetic moments distribution can be determined by integrating the majority and minority local densities of states (LDOS) up to the Fermi energy:

$$\mu_{i\alpha}=\int_{-\infty}^{\epsilon_F}[\rho_{i\alpha\uparrow}(\epsilon)-\rho_{i\alpha\downarrow}(\epsilon)]d\epsilon. \tag{3}$$

The LDOS is obtained from the diagonal elements of the Green function:

$$\rho_{i\alpha\sigma}(\epsilon)=-\frac{1}{\pi}\mathrm{Im}[G_{i\alpha\sigma,i\alpha\sigma}(\epsilon+iO^{+})]. \tag{4}$$

The diagonal elements of the Green function are calculated by using the recursion method,[19] with a sufficient number of levels in the continued fraction to assure the stability of the results. The self-consistent procedure starts with an input of $\mu_{i\alpha}$ and $\Omega_{i\alpha}$ at each site i and orbital α from which the diagonal elements of the Hamiltonian are constructed. By solving the resulting Hamiltonian with the recursion technique we obtain the LDOS. From them, a new distribution of magnetic moments $\mu'_{i\alpha}$ is obtained. The potentials $\Omega_{i\alpha}$ are also updated at each iteration. The procedure finishes when the input $\mu_{i\alpha}$ and output $\mu'_{i\alpha}$ coincide and the local neutrality condition is reached within an accuracy of 10^{-4}.

C. Transferability of the parametrization

We treat the magnetism within a molecular field model in which the spin interactions are described by the potential $z_{\sigma}(J_i/2)\mu_i$ at each atomic site i. The exchange parameter J_i has intra-atomic character, and generally it is fitted in order to recover the bulk magnetic moment.[21] In the case of the Co fcc bulk, one needs $J_{Co}=1.000$ eV to recover a magnetic moment of $1.53\mu_B$ previously determined through an *ab initio* TBLMTO method in the atomic spheres approximation (ASA).[22,23] However, the transferability of the parametrization can be improved by fitting to a system whose morphology resembles better than the bulk the system under investigation. In our case, we have chosen to fit to the single Co monolayer supported on Pd(110), because this system contains the Co-Pd interface and, at the same time, it is possible to define a simple supercell to perform an *ab initio* TBLMTO-ASA study. As in the case of the bulk, the calculations are performed using a scalar-relativistic version of the k-space TB-LMTO method with the atomic-sphere approximation. This method is based on the local-spin-density approximation[24] of the density functional theory.[25] Assuming pseudomorphic growth, the in-plane interatomic distance of Co is chosen to be the same as the calculated lattice parameter of fcc Pd. The Co-Pd interface distance is chosen as the arithmetic mean value of the calculated Co and Pd lattice parameters. The calculations are performed using an increasing number of k points, until final convergence is obtained for at least 135 k points in the irreducible Brillouin Zone. We

TABLE I. *Ab initio* TB-LMTO results for the local magnetic moments (in units of μ_B) at the Co monolayer supported on Pd(110) taken for the fit of the real space tight-binding model (TB).

Site	TB-LMTO	TB
Co	2,05	2,05
Pd1	0,28	0,48
Pd2	0,21	0,13
Pd3	0,16	0,08
Pd4	0,13	0,01

consider enough layers of empty spheres to assure that there is no interaction between the Co surfaces of adjacent supercells[26] (5 monolayers of empty spheres were enough). In Table I we report the *ab initio* TB-LMTO results for the local magnetic moments in the ground-state magnetic configuration of the single Co monolayer on Pd(110). This solution corresponds to the ferromagnetic in-plane Co overlayer. By applying now to the same system the tight-binding model with the *sp*- and *d*-electronic occupations from the TB-LMTO method, we obtain a value of $J_{Co}=0.70$ eV, which reproduces the *ab initio* value for the local magnetic moment at the Co overlayer and describes qualitatively the magnetic behavior of the Pd substrate (see Table I).[27]

In Fig. 1 we show the local densities of states at the inequivalent sites of the Co monolayer on Pd(110). It is interesting to probe that not only an integrated magnitude like the magnetic moment is reproduced through the fit, but also the densities of states are in good qualitative agreement for the chosen value of J_{Co}. The main characteristics of the LDOS are well described, in particular the large spin-splitting at the Co overlayer, the induced spin-polarization at the Pd monolayers and the location of the main peaks.

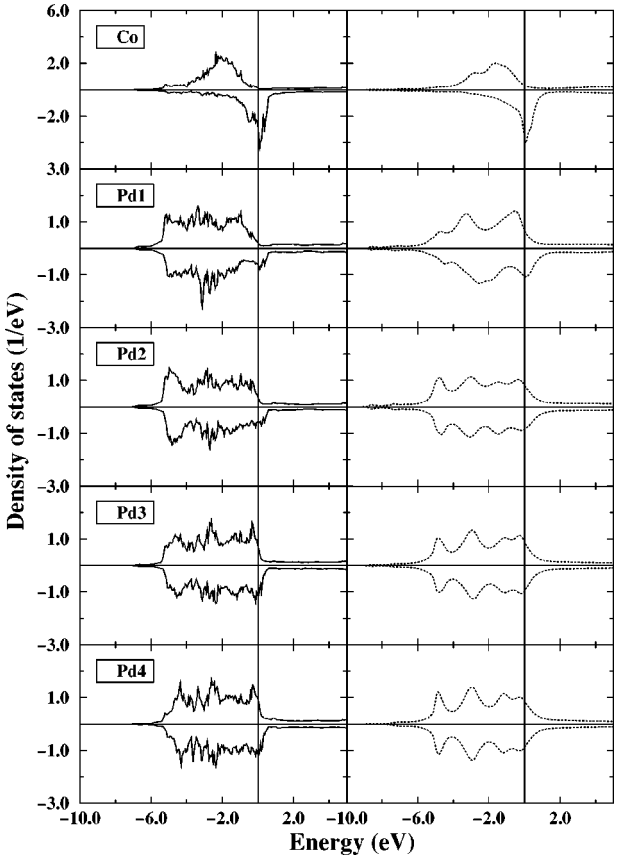

FIG. 1. Local densities of states at the inequivalent sites of the Co monolayer supported on Pd(110) obtained with both the TB-LMTO method (left column) and the TB fit (right column).

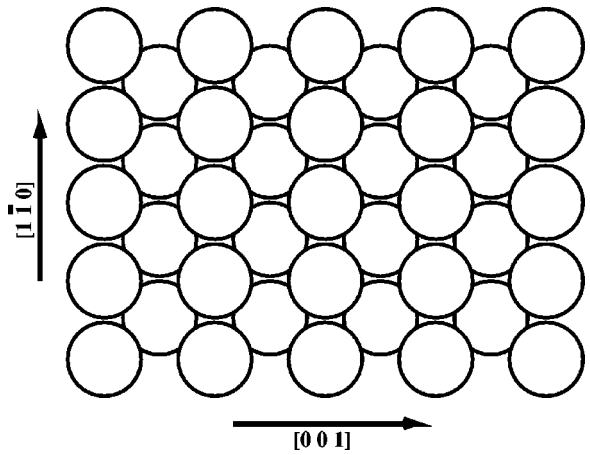

FIG. 2. View of the (110) surface of an fcc system. One can see the channels along the $[1\bar{1}0]$ direction where the atomic wires are deposited.

From Table I and Fig. 1, one can extract some general magnetic trends, which are expected to be present also in the case of supported Co wires: (i) The enhanced magnetic moment at the Co overlayer with respect to the bulk. This behavior is due to the loss of coordination at the surface giving rise to a narrowing of the DOS with the corresponding increase of the DOS at the Fermi level. (ii) The induced spin-polarization at the Pd layers in the neighborhood of Co. The absolute value of the induced magnetization in Pd is important at the interface and decreases as decreasing the hybridization with Co. However, it remains appreciable at the third Pd underlayer and it could play an important role in an indirect magnetic coupling between Co wires through the substrate. We will explore this point later on.

III. RESULTS AND DISCUSSION

The system consists of a set of monoatomic Co wires supported on the (110) semi-infinite substrate of Pd. The wires are oriented along the $(1\bar{1}0)$ direction, as we can see in Fig. 2. This is the alignment direction of the Cu wires grown and characterized by Bucher and co-workers.[10,11] The reason why the wires are aligned in this direction is that the (110) surface of a fcc system presents *channels*, where the wires are deposited. Therefore, the interwire distance can be characterized by the number of unoccupied *channels* between adjacent wires. When all the *channels* are occupied by wires we have the complete Co monolayer. We will consider this situation as the minimum interwire distance.

Let us analyze first the results for ''infinitely'' separated wires, that is the case of an isolated supported Co wire. In Fig. 3 we report the local magnetic moments at the inequivalent sites of the system. Due to the loss of neighbors, the magnetic moment of the wire is enhanced in about 8% with respect to the supported Co monolayer and much more (about 40%) with respect to the Co fcc bulk. This result was

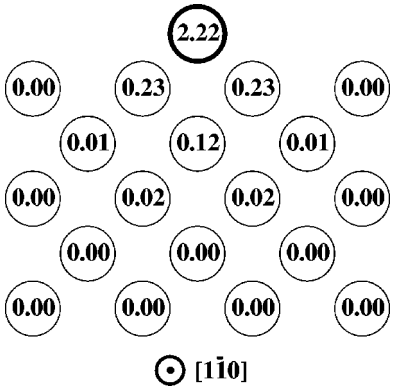

FIG. 3. Local magnetic moment distribution (in units of μ_B) for an isolated Co wire supported on Pd(110). The figure represents a cut of the system perpendicular to the $[1\bar{1}0]$ direction and the Co atoms are plotted with a thick contour.

expected as a consequence of the localization effect that takes place as going from the Co bulk to the Co monolayer and finally to the Co wire. The electronic localization is reflected in the densities of states plotted in Fig. 4. Here, it is noticeable the progressive narrowing of the DOS accompanied with an increase of the DOS at the Fermi level. At the same time, the three-peak structure characteristic of the fcc lattice is transformed in a main peak in the case of the wire, approaching the limit of magnetic saturation.

Another expected result is the spin-polarization induced by Co in the neighboring Pd atoms. It is well known that certain paramagnetic transition metals (V, Pd) can be magnetic in the presence of a strong ferromagnet. The induced spin-polarization in Pd is lower in the case of the supported wire than for the complete Co overlayer. The Pd layer at the interface with the Co overlayer displays a magnetic moment of $0.48\mu_B$, whereas the nearest Pd neighbor of the Co wire only has $0.22\mu_B$. This is a consequence of the reduction of the Co-Pd hybridization when the Co coordination of the Pd sites decreases as going from the overlayer to the wire configuration. Previous *ab initio* Korringa-Kohn-Rostoker calculations for a dilute Co atom-impurity embedded in Pd bulk have also shown this effect.[28] In this case, the induced spin-

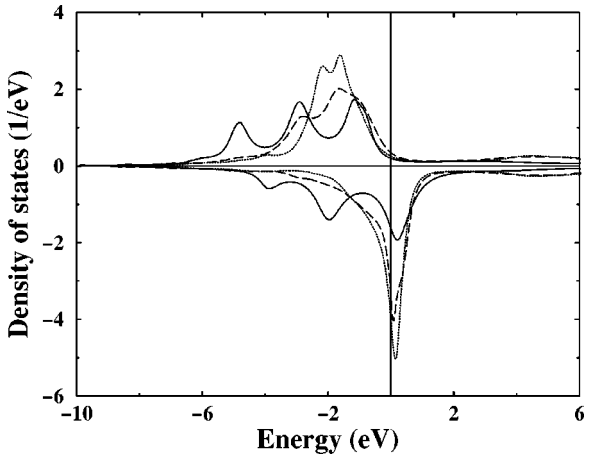

FIG. 4. Densities of states obtained for Co fcc (solid line), the Co monolayer supported on Pd(110) (dashed line) and the isolated Co wire supported on the same substrate (dotted line).

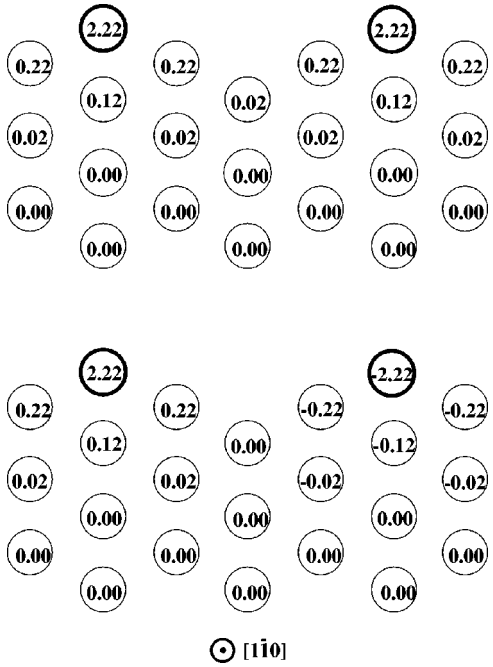

FIG. 5. Local magnetic moment distribution (in units of μ_B) for the *P* solution (upper half) and the *AP* solution (lower half) of the supported Co wires separated by one channel.

polarization in Pd is even lower than for the supported wire system due to the extremely low Co-Pd hybridization (only one Co atom surrounded by Pd).

Although the induced magnetic moment in Pd is relatively small, one open question is if the Co wires can interact magnetically through the Pd substrate, that is, if there exists an indirect magnetic interaction between the Co wires (as well as the possible direct magnetic interaction if they are close enough). This question can be answered after calculating the magnetic moments distribution when the interwire distance is reduced and the Co wires approach each other. Besides, it is worthwhile to compare different possible magnetic configurations, in particular two: adjacent Co wires with either parallel (*P*) or antiparallel (*AP*) magnetic coupling.

Figure 5 reports the magnetic moment distribution of both *P* and *AP* solutions for the supported Co wires separated by one channel. For this interwire distance, the resulting values for the local magnetic moment at the Co atoms are similar to those found in the case of the isolated wire. Furthermore, the absolute values in both *P* and *AP* configurations are also similar, an exception being those Pd sites in the *AP* configuration located at the same distance of both the wire with positive magnetic moment and the wire with negative magnetic moment. Those Pd atoms are magnetically frustrated (they have $0\mu_B$). This result indicates that at this interwire distance, the magnetic interaction between wires (both direct and indirect via the Pd substrate) is negligible. If magnetic interactions took place, two behaviors were expected. On the one hand, the local magnetic moments at the Co wires in the *P* solutions should reduce and converge to the corresponding value in the supported overlayer ($2.05\mu_B$). On the other hand, since Co is a strong ferromagnet, the *AP* solution should become less stable than the *P* solution. Neither of these effects are present for this interwire distance.

The closest possible interwire distance corresponds to the

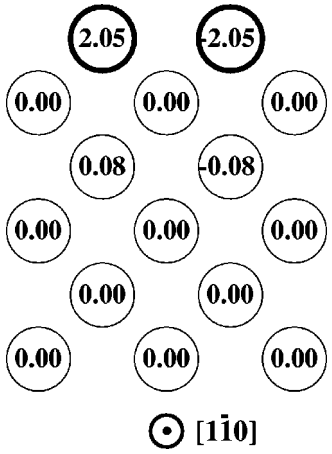

FIG. 6. Local magnetic moment distribution (in units of μ_B) for the AP solution of the supported Co wires in their closest position that corresponds to the Co monolayer.

complete Co overlayer. We have already calculated the P solution, which corresponds to the ferromagnetic-in-plane solution of the Co overlayer (see Table I). However, it is interesting to check if it is possible to obtain the AP solution in this case. The answer is positive. Figure 6 shows this solution. The absolute values for the local magnetic moments at the Co sites are the same for both P and AP configurations. Besides, the energy difference per atom between both solutions is small ($E_P - E_{AP} \approx -25$ meV). Although the P solution is more stable, this energy difference is about half the room temperature. This result indicates that the magnetic interaction between the Co wires, although it exists, is small. For the AP solution the induced magnetic moment in Pd is negligible due to the frustration effects and the average magnetic moment of the system is zero. In summary, since Co moments reduce from $2.22\mu_B$ to $2.05\mu_B$ as going from separated wires to the overlayer, the magnetic interaction starts only when the intrawire distance approaches 3.89 Å, that is the corresponding distance in the Co overlayer. The reason why the magnetic interaction is small is double. First, in the (110) crystallographic orientation, the distance between the wires (even in the closest configuration) is larger than the distance between adjacent Co atoms inside the wire. Second, the lattice parameter of Pd fcc (3.89 Å) is larger than the lattice parameter of Co fcc (3.46 Å). Both facts give rise to a minimum wire-wire distance of 3.89 Å(the distance in the overlayer assuming the pseudomorphic growth), and this distance is much larger than the nearest-neighbor distance in Co fcc (2.45 Å).

IV. SUMMARY

We have calculated the local magnetic moments distribution of monoatomic Co wires supported on Pd(110) for several interwire distances. The morphology of the system is modeled following the experimental results of Bucher and co-workers[10,11] for Cu wires on Pd(110). The exchange parameter of our self-consistent tight-binding model, as well as the *d*- and *sp*-electronic occupations, have been fitted to *ab initio* TB-LMTO results previously obtained for the ferromagnetic-in-plane solution of the Co monolayer deposited on the same substrate. The main results are

(i) The magnetic moment of an isolated supported wire is enhanced in about 8% with respect to the supported Co monolayer and in about 40% with respect to the Co fcc bulk. This trend is due to the electronic localization effect.

(ii) There exists an induced spin-polarization in the Pd atoms close to the Co wire due to Co-Pd hybridization. This induced magnetic moment in Pd is lower than the one obtained in the case of the complete Co overlayer, but larger than the one reported[28] for a single dilute Co impurity in the Pd fcc bulk. This trend is due to the different degree of Co-Pd hybridization in those systems.

(iii) The magnetic interaction between adjacent wires starts only when the intrawire distance approach 3.89 Å, that is, the interwire distance for the complete supported Co monolayer. This magnetic interaction is, however, small. The AP solution persists even in the case of the supported Co monolayer with absolute values for the local magnetic moments in the Co sites similar to those of the P solution. Besides, the energy difference per atom between the AP configuration and the ground-state P configuration is about half the room temperature.

In view of the possible technological applications, our results show that it is possible to optimize an assembly of Co wires supported on Pd(110), since they preserve their intrinsic magnetic moment (nearly saturated) for interwire distances close to the monolayer regime. Besides, it has been recently predicted perpendicular magnetic anisotropy[15] in a supported Co wire. This opens also the possibility of using these new systems for magneto-optic purposes.

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