Magnetocrystalline anisotropy of Co-Pd interfaces

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(Received 14 June 1993)

The interface magnetocrystalline anisotropy (MCA) of a Pd/Co/Pd sandwich is calculated by employing the recently proposed state-tracking approach and the full-potential linearized augmented-plane-wave energy band structure. The strong positive (perpendicular) Co-Pd interface MCA arises from the hybridization between the out-of-plane Co bonding $xz(yz)$ states with the interface Pd atom: the large d-d bonding strength and high energy of the Pd d states shifts a substantial component of these Co states (bands) above the Fermi energy. Comparisons with a previous study on the Co-Cu interface makes clear that the difference between the effects of two groups of substrates (Cu, Ag versus Pd, Au, etc.) depends on the interface bonding strength and the position of the d states of the interface atoms—as is qualitatively revealed by an analysis based on the use of an effective ligand-interaction model.

I. INTRODUCTION

Recent experiments have revealed that strong perpendicular magnetocrystalline anisotropy (MCA) occurs due to the existence of the interface in $X/\mathrm{Co}/X$ multilayers, where X denotes the usually nonmagnetic substrates. When X=Pd, Pt, Au, and Ir, an interface anisotropy (corresponding to $2K_s$ in the literature) of about 1.0–1.6 mJ/m^2 ($\sim$ 0.34–0.54 meV/atom) was observed for these multilayers. Perpendicular magnetization is realized in these systems when the thickness of the Co layer is 1–2 monolayers (ML) and this positive interface anisotropy dominates the volume demagnetization contribution.[1] Thus, they are promising candidates for high-density magneto-optical storage media, and have attracted a great deal of attention. By contrast, for X=Cu and Ag, $X/\mathrm{Co}/X$ multilayers all showed in-plane easy magnetization, though a faint positive value of the interface anisotropy was also reported from an extrapolation of the data for thicker Co layers.[1]

First principles calculations of the MCA of $X/\mathrm{Co}/X$ (111) multilayers was reported for X=Cu, Ag, and Pd by Daalderop *et al.*,[2] which showed a strong positive interface MCA for Pd/Co/Pd multilayers (0.3–0.8 meV), but weak MCA for Cu/Co/Cu (0.2 meV/atom) and Ag/Co/Ag (0.15–0.25 meV/atom) multilayers, in reasonable agreement with available experiments. However, the relationship between the interface MCA and the electronic structure was not made clear, because the calculated results were based on integration over the Brillouin zone (BZ) of the contributions which exhibit very strong random fluctuations.[3] Hence, while the strong dependence of the interface MCA of the $X/\mathrm{Co}/X$ multilayer films on the atomic species of the substrate layer X is well recognized from both experiment and theoretical calculations, the difference between the two groups of substrates has never been explained satisfactorily.

The interface MCA has been considered as a sum of two contributions.[1] The first is the Neél term $K_N = \sum L \cos^2\theta$, which expresses the total MCA as a sum of pairwise contributions. It is only a phenomenological description since it does not account for how the value of L depends on the atomic species. The second term is a contribution from the misfit strain anisotropy which exists when the magnetic and substrate layers are incoherent.[4] This term is also hard to use to account for the difference between these two groups of atomic species; for example, both the Co-Cu (smallest mismatch) and Co-Ag (largest mismatch) belong to the same group.[2]

It was shown in our recent papers[5–7] that there is a close relationship between the electronic structure and the MCA for a system with reduced symmetry: For example, the dominant contribution to the strongly negative interface MCA of a free standing Co monolayer is determined mainly by the spin-orbit coupling (SOC) between antibonding z^2 and bonding $xz(yz)$ states near $\overline{M}$.[5,7] We also showed that at the Co-Cu interface, this MCA contribution has been drastically decreased in magnitude, in agreement with experiment,[8] because the bonding $xz(yz)$ Co states are directed out of plane, are close in energy to the interface d states, and thus interact strongly with the interface Cu states.[7]

An effective-ligand-interaction model (ELIM) was developed for the interpretation of the first principles results of the Co-Cu interface effect on the MCA. Analysis of this model showed that the interface bonding strength

and the position of the energy of the interface d states determine the intensity and direction of the change of the interface MCA.[7] While this idea explained qualitatively the difference between those two groups of substrates, it needs to be examined by first principles calculations.

This paper presents the results of a first principles investigation of the MCA of the Co-Pd interface. After a description of the method used in our investigation in Sec. II, the electron states at the Co-Pd interface obtained with our highly precise full-potential linearized augmented-plane-wave (FLAPW) method[9] is discussed in Sec. III. The resulting MCA and interface effect are given in Sec. IV, with a discussion about the contribution from both Co and Pd atoms. Section V compares our results with experiment and previous theoretical calculations, and provides a summary of our investigations.

II. METHODOLOGY

To demonstrate the interface effect, a Co monolayer sandwiched between a Pd(001) slab represented by two Pd layers (a total of five layers) is used as our model system. While relaxation may exist at the interface, as shown in previous theoretical investigations,[10] no experimental data are available as yet. For showing the role of the electronic properties of the interface atoms on the effects on the MCA, we set at present the geometry of the sandwich identical to an ideal fcc Pd(001) five-layer slab; i.e., the same interplane distance for Co-Pd planes as that for Pd-Pd planes is used in present study. The z axis is defined as the layer normal, and directions x and y are in the layer plane and along the lines connecting the nearest neighboring atoms.

More than 60 plane waves per atom are used as the variational basis set to solve the semirelativistic Kohn-Sham equations in the FLAPW calculation. Within the muffin-tin spheres, lattice harmonics with angular momentum l up to 8 are used to expand the charge density, potential, and wave functions. For generating the charge density, integrations over k space are replaced by summations over 15 special k points in the 1/8 irreducible two-dimensional BZ, i.e., 100 k points in the full BZ. Convergence is assumed when the average root mean square deviation between the input and output charge densities is less than $1 \times 10^{-3}\ e/(\text{a.u.})^3$, and the deviation between spin densities is less than $3 \times 10^{-5}\ e/(\text{a.u.})^3$.

The single state energy shifts induced by the SOC are calculated in a second variation approach, with all states in the range up to 13 eV above E_F included in the variational basis.[11,12] The SOC Hamiltonian matrix elements are calculated by integrating the derivative of the spherical potential over the muffin-tin region of the Co and/or Pd atoms, and the contributions from the interstitial and vacuum regions are neglected—as was done previously.[6] A perturbative (rather than self-consistent) treatment based on a force theorem[13] is adopted, in which the SOC-induced change of the total energy is approximated by the difference of the single state energies summed over all occupied states. The state-tracking approach was adopted to determine the perturbed set of occupied states,[12] which ensures that the resultant MCA reflects solely the physical effect of the SOC, free from random fluctuations obtained by the usual Fermi filling of states in the non-self-consistent perturbation calculations. For calculating the SOC-induced change in the total energy, integrations were performed over 66 k points in the 1/8 irreducible two-dimensional BZ (corresponding to 400 k points in the full BZ); the SOC-reduced symmetry in the xy plane is considered by summing over appropriate operations of the moment direction in the plane.

III. ELECTRON STATES AND SPIN POLARIZATION

The calculated density of states (DOS) is plotted for the Pd/Co/Pd sandwich in Fig. 1, and compared with

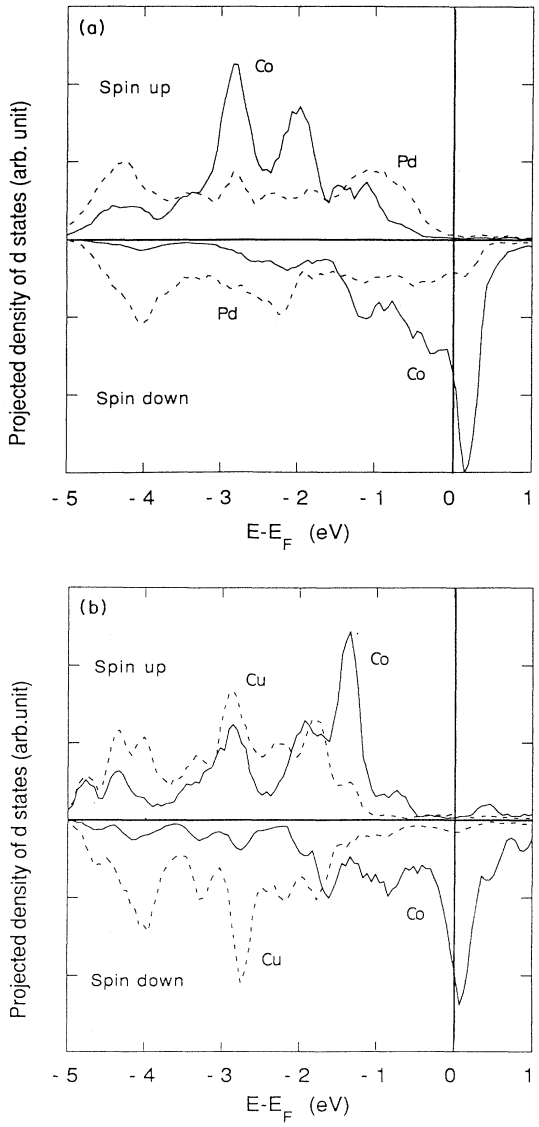

FIG. 1. Density of states of (a) the Pd/Co/Pd (001) sandwich and (b) the Cu/Co/Cu (001) sandwich. Solid lines are layer projected Co d states, and dashed lines are layer projected interface Pd(Cu) d states.

that for the Cu/Co/Cu sandwich, which was thoroughly studied for its MCA properties previously.[7] The projected density of states is shown for the Co and interface Pd(Cu) layers. The average d band energy ϵ_d, bandwidth, and exchange splitting are listed in Table I for both Pd/Co/Pd and Cu/Co/Cu.

Strong hybridization between the Co and Pd spin-down bands is clearly seen in Fig. 1(a) in the energy range between −1.5–0.5 eV with respect to the Fermi energy. The reason for the strong interaction in the Co-Pd system is the reduced localization of the Pd 4d orbitals. Because of this interaction, stronger spin polarization of the Co d bands and magnetic moment for the Co atom at the Co-Pd interface larger than that of the Co-Cu interface are clearly seen in Table I, as already recognized previously.[10,14]

By contrast, the interface Cu d states have more localized orbitals and lower energy (−2.12 eV below that of Co spin-down d bands). Thus, the Co and Cu d orbitals have less overlap, and the effect of the hybridization between the spin-down Co and Cu d bands is much weaker. However, there is an appreciable component of the Co d states which has been brought to lower the energy range (about −2 to −3 eV below E_F).

As pointed out in our previous paper,[7] for understanding the interface MCA the most crucial factor is seen in the change of the out-of-plane d states. For this purpose, we plot Figs. 2(a) and 2(b) which compare the hybridization of the Co d states at the Co-Pd and Co-Cu interfaces at $\overline{\Gamma}$ and $\overline{M}$, respectively. The difference in the change of the out-of-plane $xz(yz)$ states is noticed most remarkably. At $\overline{\Gamma}$ [Fig. 2(a)], the out-of-plane $xz(yz)$ are antibonding and lie above E_F. At the Co-Cu interface their changes are very small due to the large energy separation between these out-of-plane Co antibonding states and the Cu d states. By contrast, at the Co-Pd interface they exhibit appreciable hybridization because the energy of the Pd d states is higher and thus closer to these antibonding out-of-plane Co states. The strongest interface interaction happens to the bonding $xz(yz)$ Co state at $\overline{M}$ [Fig. 2(b)] because its energy is close to the interface Pd(Cu) d states. A substantial component [53%; see Fig. 2(b)] of the Co d wave function of these bonding states is now in the hybridized states which are shifted upward by about 0.7 eV, and already located slightly above E_F [Fig. 2(b)].

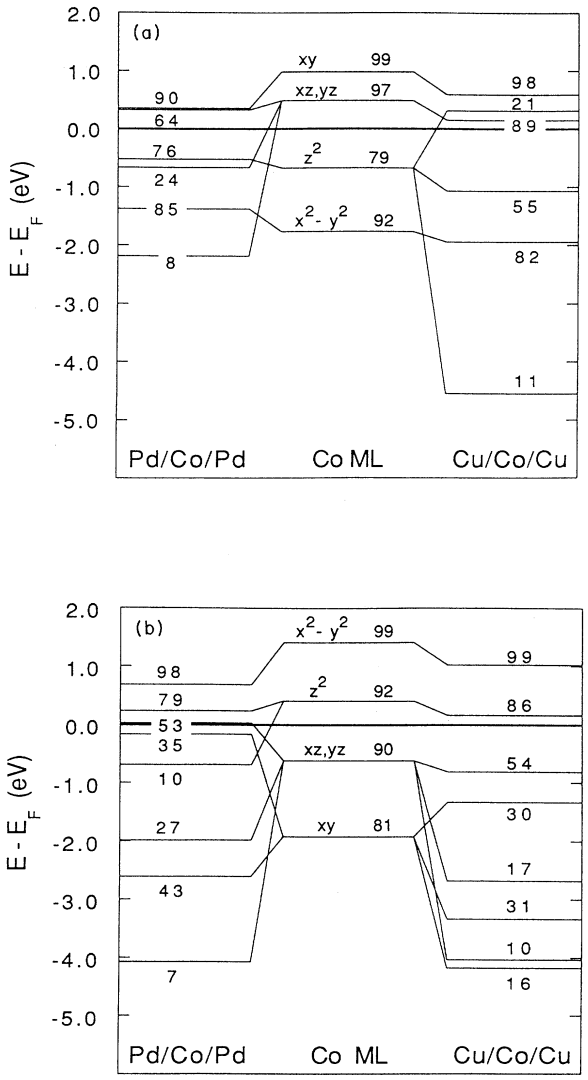

FIG. 2. Comparison of the effect of the Co-Pd and Co-Cu interface on the Co d electron states (a) at $\overline{\Gamma}$ and (b) at $\overline{M}$. Numbers are the percentage of the Co d components inside the Co muffin-tin spheres.

TABLE I. Average energy of d states, ϵ_d, and their bandwidth W (determined from the density of states curves), exchange splitting ΔE_{ex} (difference between ϵ_d for spin-up and spin-down bands), and magnetic moments m of Pd/Co/Pd and Cu/Co/Cu (001) sandwiches. The lattice constant a is given as the distance between nearest neighbor atoms.

System	Atom	ϵ_d (eV) spin-up (down)	W (eV) spin-up (down)	ΔE_{ex} (eV)	m (μ_B)
Pd/Co/Pd (a =5.24 a.u.)					
	Co	−1.91 (0.05)	2.56 (2.63)	1.96	2.09
	Pd(i)	−1.61 (−1.38)	3.60 (3.62)	0.23	0.37
	Pd(s)	−1.06 (−0.91)	3.14 (3.12)	0.15	0.20
Cu/Co/Cu (a=4.83 a.u.)					
	Co	−2.11 (−0.58)	3.01 (3.16)	1.53	1.69
	Cu(i)	−2.77 (−2.70)	2.69 (2.74)	0.07	0.05
	Cu(s)	−2.22 (−2.21)	2.34 (2.34)	0.01	0.01

By contrast at the Co-Cu interface, since the Cu d states are lower in energy, these out-of-plane Co bonding states are shifted to lower energies [Fig. 2(b)] due to their hybridization with the interface Cu d bands.

The general trend of this change in energy and hybridization due to the interface interaction was expected from the effective-ligand-interaction model (ELIM) given in our previous paper.[7] There, tabulated empirical data given by Harrison[15] were used for the relevant parameters. According to Harrison, the Pd-Pd d bonding strength is stronger than Co-Co bonds, and the Cu-Cu d bonding is the weakest (given by the r_d values in the "Solid State Table"[15]). This is also verified by our first principles results as shown by the the small Cu d bandwidth and large Pd d bandwidth in Table I. The position of the d states estimated from those empirical parameters is also in qualitative agreement with the present first principles results: The values $\epsilon_d(X) - \epsilon_d(\mathrm{Co})$ estimated for spin-down states are -0.7 and -3.2 eV for X=Pd and Cu, respectively,[7] which compares with -1.43 and -2.12 eV given in Table I for the energy difference between the interface Pd(Cu) and Co states.

IV. MAGNETOCRYSTALLINE ANISOTROPY

The SOC-induced energy $E^{sl}(\sigma)$ is calculated for two directions of magnetization, i.e., when the magnetization is parallel to z and x. The anisotropy energy ΔE^{sl} is given as $\Delta E^{sl} = E^{sl}(x) - E^{sl}(z)$. Because ΔE^{sl} depends on the band filling, we change the band filling by varying the highest occupied energy E around the physical value of E_F in a rigid band calculation to reveal the contribution from the SOC between different bands.[6] We plot the variation of the MCA energy either as a function of the number of the valence electrons, Z, usually when comparing different systems, or against the highest occupation E when comparison is made on the same system.

A. Contribution from the Co SOC

Figure 3 gives the band filling dependence of the MCA of the Pd/Co/Pd sandwich (solid line) calculated by including only the SOC inside the Co muffin-tin sphere and neglecting that of the Pd. For comparison, also shown is the curve (long dashed line) for a free standing Co monolayer which exhibits the band filling dependence typical for $3d$ transition metal monolayers. It is characterized by the strong negative peak at about half-occupation of the spin-down d band and a change of the MCA sign at slightly less occupation.[6]

Obviously, for Pd/Co/Pd the negative peak of the MCA is still as strong as for a free standing monolayer, but its position has been largely shifted to the larger band filling region. This behavior is caused mostly by the change of the upward shift of the out-of-plane $d_{xz,yz}$ bands as shown in Fig. 2(b). As a result, the large negative contributions to the MCA energy from the SOC between the $d_{xz,yz}$ and d_{z^2} states around $\bar{M}$, which plays the key role for the negative MCA energy for the Co monolayer,[5] are significantly reduced. A positive MCA

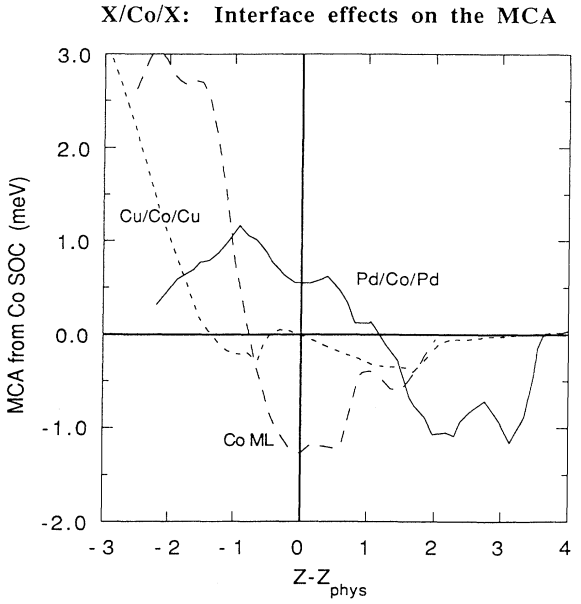

FIG. 3. Comparison of the effect of the Co-Pd and Co-Cu interface on the MCA contribution calculated when only the SOC inside the Co muffin-tin spheres is included. Results are plotted as a function of the number of valence electrons by a rigid band calculation. Long dashed, short dashed, and solid lines are for Co ML, Cu/Co/Cu, and Pd/Co/Pd sandwiches, respectively. (A Gaussian broadening with full width 40 meV was employed.)

contribution from the SOC of the Co layer, 0.55 meV per Co atom, is thus achieved at the physical value of band filling.

This behavior is in some sense very similar to the origin of the positive MCA of a free standing Fe monolayer: Most of the bonding $xz(yz)$ bands become empty due to the change of the position of E_F with respect to the $xz(yz)$ bands. In the case of a free standing Fe monolayer, this change is due to the reduction of the the number of valence electrons, but at the Co-Pd interface, it is due to the upward shift of the bonding $xz(yz)$ states.

This behavior is in clear contrast to the behavior of the Co-Cu interface, where the magnitude of the negative MCA peak is greatly reduced and the change of MCA sign is shifted to less band filling region (short dashed line in Fig. 3) due to the downward shift of the out-of-plane bonding bands [Fig. 2(a)].

We have previously discussed this mechanism using the effective-ligand-interaction model (ELIM)[7] which attributes the difference between two groups of substrates (Cu and Ag versus Pd and Au) to the different d bonding strengths and energies of their d states. The present first principles calculation shows that the idea proposed in the ELIM qualitatively describes the main features of this effect on the interface MCA.

Finally, consider possible effects caused by changes in the SOC constant. It turns out that the SOC constant for Co atoms remains almost unchanged to within ± 3% in either isolated monolayers (shown in Table II for different lattice constants), or in layers adjacent to either a Cu or

TABLE II. Spin-orbit coupling constants (radial integration) ξ, theoretical value of the MCA, ΔE^{sl}, of X/Co/X (001) sandwiches, and experimental interface MCA values $2K_s$. The lattice constant a is given as the distance between nearest neighboring atoms.

System	Atom	ξ (meV) spin-up (down)	ΔE^{sl} (meV) present	references	$2K_s$ (meV)
Pd/Co/Pd (a=5.24 a.u.)			0.23–0.68	0.85[a]	0.43[b]
	Co	41.0 (37.8)	0.55		
	Pd(i)	112.4 (111.1)			
	Pd(s)	111.6 (111.1)			
Cu/Co/Cu (a=4.83 a.u.)			−0.01	0.20[a]	0.10[c]
	Co	39.6 (37.1)	−0.01		
	Cu(i)	59.0 (58.9)			
	Cu(s)	58.7 (58.8)			
Co monolayer					
(a=4.83 a.u.)	Co	40.0 (37.2)	−1.35		
(a=5.45 a.u.)	Co	39.2 (36.9)	−2.59	−3.6[d]	

[a]Reference 2 for X/Co/X (111) multilayers.
[b] Reference 17.
[c] Reference 8.
[d] Reference 18.

Pd substrate. Also, the difference of the SOC constants between spin-up and spin-down states is different by only about ± 5% for the strongest spin-polarized Co atoms, because the calculation of the radial integral in the SOC Hamiltonian matrix elements includes the contribution of the exchange potential. Both these changes, however, should not have any appreciable effect on the MCA.[16]

B. Contribution from the SOC of substrate Pd(Cu) atoms

In the Cu/Co/Cu sandwich, the spin polarization of the Cu bands is small [Fig. 1(a)], and the MCA contribution of including the SOC inside the Cu muffin-tin region was found to be negligible.[7] However, in the case of Co-Pd, the strong exchange interaction produces an appreciable spin polarization, with $m = (0.20\text{–}0.37)\mu_B$, on the Pd atom (see Table I) which is about one-tenth to one-fifth of the moment of the Co atom. At the same time the SOC constant of the heavier Pd atom is about 3 times larger than that for the 3d elements (Table II). The MCA, as a second order effect of the SOC perturbation, is approximately proportional to the square of the product of the magnetic moment and the SOC constant. Therefore, while the contribution to the MCA of the substrate Pd atoms is expected to still be less than the Co layer, it would no longer be negligible.

The results of the MCA contribution (per Pd atom) calculated when only the SOC of the Pd atoms is included are shown in Fig. 4 by the solid line. Obviously, the magnitude of this contribution is less than that from the Co SOC (long dashed line in Fig. 4) in accordance with above reasoning, but certainly cannot be simply omitted as in the case of the Cu substrate. Since in the structure employed each unit cell contains four Pd atoms (versus one Co atom), the contribution from the Pd SOC becomes even more prominent in determining the total MCA (per unit cell).

The total MCA calculated with the SOC in both Co and Pd muffin-tin spheres included is shown in Fig. 4 by the short dashed curve. It is not simply the sum of the two contributions of including Co or Pd SOC separately, because the MCA comes from the second order SOC perturbation, cross terms should exist too. Note that the general trend of the variation of the total MCA with respect to the band filling follows approximately the curve of the contribution from the Co SOC only. This shows that the magnetic Co layer plays the most im-

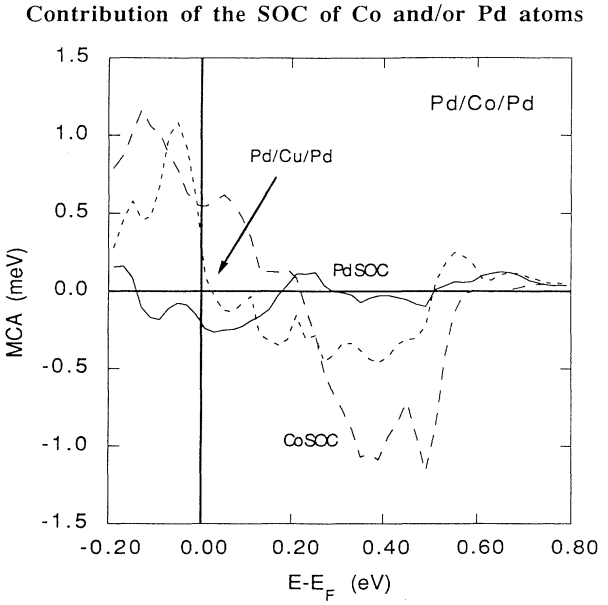

FIG. 4. MCA of the Pd/Co/Pd (001) sandwich (solid line), the contribution of the Co SOC (long dashed line), and the contribution (per Pd atom) of the Pd SOC, plotted as a function of the highest occupation energy. (A Gaussian smooth with full width 40 meV was employed.)

portant role in determining the MCA behavior of this interface, although inclusion of the Pd SOC does make a difference. The resultant MCA becomes 0.23 meV (per unit cell) compared to 0.55 meV when only the Co SOC is considered.

C. Uncertainty due to surface pair coupling

It was shown that singularity due to a quasidegenerate pair of occupied and empty states near the E_F which occurs when two bands intersect at the Fermi surface causes error in the non-self-consistent calculation of the SOC-induced change of the total energy.[6] When the large SOC constant of the heavier Pd $4d$ atoms is included, the effect of the singularity caused by this surface pair coupling (SPC) on the calculated MCA becomes more influential. A non-self-consistent calculation is expected to overestimate the MCA contribution of the SPC, and in a discrete mesh integration with a limited number of k points the error due to this singularity is larger.[6] In the present case, a force theorem calculation integrated over 66 k points, it may at most lead to an uncertainty in the magnitude of 110/66–2 meV.

An estimate of the possible error due to this singular contribution is made in Fig. 5, where the dashed and solid lines are calculated including the SOC of both Co and Pd atoms, when the SOC between the surface pairs is included and omitted by a decoupling approximation, respectively. In this decoupling approximation,[6,12] whenever the energy difference of a pair of occupied and empty states is less than the largest (among all magnetization directions) SOC, i.e.,

$$\epsilon_u - \epsilon_o < \text{Max } |\langle o|H^{sl}(\sigma)|u\rangle| \quad , \tag{1}$$

the contribution of this pair is omitted in the calculation

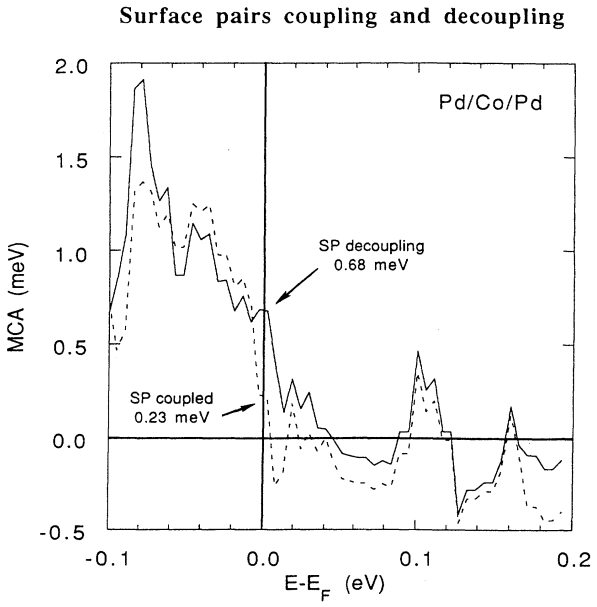

FIG. 5. The MCA of the Pd/Co/Pd (001) sandwich calculated when surface pair coupling is included (dashed line) or excluded (solid line).

of the SOC energy for all magnetization orientations (by setting this matrix element to zero in the second variation calculation of the single state SOC shift).

Obviously, the two curves in Fig. 5 exhibit the same behavior, which shows that the MCA is not mainly determined by the surface pairs, and the physical picture given in preceding sections does not depend on them. However, at given value of band filling, the MCA value changes appreciably, and bears an uncertainty up to about ± 0.2 meV. By contrast, for $3d$ systems[5–7,12] the error due to this singularity is ± 0.1 meV, because their SOC constants are smaller. For example, at the physical band filling of the Pd/Co/Pd sandwich, the MCA is changed from 0.23 meV value obtained including the surface pair coupling to 0.68 meV when the surface pairs are decoupled. In Table II both values are given as an estimation for the lower bound (surface coupling included) and the upper bound (surface coupling excluded) of the MCA and compared with experiment.

V. DISCUSSION AND CONCLUSIONS

In the experiments, the interface MCA is determined for either multilayer films or for a single magnetic film (overlayer or sandwich). In both cases, the measurements are made over a thickness range of the magnetic Co layers from often slightly larger than one monolayer to a few tens of monolayers. The interface MCA is obtained by an extrapolation to zero thickness in order to substract the volume contribution (demagnetizion and bulk magnetocrystalline anisotropy). In this procedure, the resultant interface anisotropy is best considered as the sum of two equivalent Co-X interfaces, and usually indicated as $2K_s$ in the literature.[1] At present, we make a comparison of the interface MCA, ΔE^{sl}, with the experimentally determined $2K_s$ values, for the sandwiches with a single Co monolayer (thus a X-Co-X interface) and leave the question of possible variation with thickness of the magnetic layer to later investigations.

Engel *et al.*[17] showed that the interface MCA of a Pd/Co/Pd multilayer is 0.43 meV, for (001), (110), (111) epitaxial films and polycrystalline substrates. Our results, ΔE^{sl} = 0.23–0.68 meV, are in good agreement with their experimental value (Table II). Our results for the Co-Cu interfaces also agree with the measurement by Krams *et al.*[8] for a single Co overlayer on the Cu(001) substrate (with Co layer thickness down to 1.6 ML), and the Cu/Co/Cu (001) sandwich with Cu cover layer (Table II).

Theoretical calculations by Daalderop *et al.*[2] for Pd/Co/Pd and Cu/Co/Cu (111) multilayer films showed that the strongest interface anisotropy always happens for the thinnest (monolayer) magnetic layer. Their results are about 0.2 meV more positive than ours for both Pd/Co/Pd and Cu/Co/Cu cases (cf. Table II). The slight difference may be due to (a) a difference between sandwich and multilayer films; (b) the crystallographic orientation of the substrate; (c) lattice relaxation, which was considered by Daalderop *et al.* in a constant volume approximation, but neglected in present paper; or (d) a difference in the band methods and integration over

k space (state tracking vs "blind" Fermi filling), considering also the error bars in the calculations, which are estimated in our calculation as ± 0.1 meV (Cu/Co/Cu) or ± 0.2 meV (Pd/Co/Pd), and were given as ± 0.1 meV in Ref. 2. The difference is quite reasonable.

It is worth pointing out that the use of our state-tracking approach has reduced the integration mesh for this sandwich also to only 400 k points over the full Brillouin zone, the same as for a monolayer film, in contrast to the more than 1000 points used for either monolayer or multilayer calculation.[3,2] The complexity in the band structure of a sandwich film does not lead to any additional problem when the state-tracking approach is adopted.

Despite the fact that an ideal structure was used in present study, the agreement between our results and the experiment, and also the approximate agreement between our results and the multilayer calculation,[2] indicate that the interaction between the magnetic and interface atoms plays the most important role in determining the interface MCA. The origin of the strong positive (perpendicular) Co-Pd interface MCA was shown to be due to the hybridization between the out-of-plane Co bonding $xz(yz)$ states with the interface Pd atom. The large d-d bonding strength and high energy of the Pd d band cause a substantial component of these Co states (bands) to be shifted to above the Fermi energy, and the SOC between these states and the empty z^2 states (bands) no longer contributes (negatively) to the MCA. The difference between the two groups of substrates (Cu, Ag versus Pd, Au, etc.) was also made clear to depend on the interface bonding strength and the position of the d states of the interface atoms, as first qualitatively revealed in the effective-ligand-interaction model analysis.[7]

Although the induced magnetic moment is not very large on the Pd atoms ($\sim 0.3\mu_B$/atom) at the Co-Pd interface, the large SOC of the heavier 4d Pd atoms does contribute appreciably to the total interface SOC. In this case, the large SOC also leads to larger uncertainties in the determination of the MCA due to the surface pair coupling ($\sim \pm 0.2$ meV). An interesting case would be for the Co-Pt and other 5d metal (also 5d noble metal Au) interfaces. While even stronger bonding occurs for 5d elements and positive interface MCA is thus expected in accordance with experimental evidence of positive MCA of Co-Pt, Co-Ir, and Co-Au multilayers, theoretical treatment for the case when the SOC becomes comparable to that of the crystal field strength requires more considerations.

The results of free standing Co monolayers are also given in Table II for two lattice constants. It is obvious that over this large range of lattice constant, free standing Co monolayers show in-plane anisotropy. Hence, the strong positive interface MCA in Pd/Co/Pd is obviously not due to a strain effect. However, in the case of epitaxy, larger substrate lattice constants would most probably lead to a contraction of the distance between the magnetic layer and the lattice plane of the interface atoms, and a contraction as large as 5–6 % was expected at the Co-Pd interface for Co on a Pd(111) overlayer.[10] This will certainly enhance the interface d-d interaction, and the MCA is expected to become more positive as given by the effective-ligand-interaction model.[7] Though qualitatively the physical picture of the strongly positive MCA of Pd/Co/Pd interface MCA is not expected to be changed by including this relaxation, it is needed certainly in a quantitative theoretical determination, and this structural relaxation should also be noticed in the experiment.

ACKNOWLEDGMENTS

Work at Northwestern supported by the National Science Foundation (Grant No. DMR 91-17818 and a grant of computer time at the Pittsburgh Supercomputing Center through its Division of Advanced Scientific Computing). One of us (D.S.W.) acknowledges the support of the National Science Foundation of China.

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