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Interface magnetism in ultrathin Fe/W(110) films from first principles

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An *ab initio* study of the magnetic properties of Fe ultrathin films on top of a W(110) substrate shows that for one Fe layer the magnetization axis is in-plane. For an additional layer of Fe, the magnetosurface and magnetoelastic anisotropies favor a magnetization axis perpendicular to the substrate, but the total energy including the shape anisotropy is minimal for the spin axis in-plane. In the case of the trilayer film all anisotropies favor an in-plane magnetization axis. The spin magnetic moment of the first Fe atomic layer is close to the bulk value while that of the second and third Fe atomic layers are considerably increased. The W atoms at the interface are weakly antiferromagnetically coupled to Fe. The orbital magnetic moment anisotropy of all the atoms is shown to be directly related to the calculated x-ray magnetic circular dichroism anisotropy.

I. INTRODUCTION

Low-dimensional systems like surfaces and films have attracted a lot of attention during the last few years, principally because of the enhancement of their magnetic properties. The explanation of these properties can lead to a deeper understanding of the mechanisms that govern the magnetic anisotropy and its connection to the magnetic moments of the atoms. Films of $3d$ metals on a paramagnetic substrate are one of the most studied cases, and especially Fe layers on top of a W substrate have served as a model system during the last years.

The interest on ultrathin films of Fe/W(110) is limited to films up to two Fe monolayers because thicker Fe films show ferromagnetism but no striking properties.[1] In the submonolayer region, Fe islands on W(110) show a superparamagnetic behavior, except for a very narrow area around 0.24 ML for which magnetic percolation occurs and ferromagnetism appears.[2] Fe monolayer on W(110) is thermodynamically stable,[3] and as shown by Mössbauer experiments the first monolayer of Fe grows pseudomorphically on W(110).[3,4] This was recently verified by scanning tunneling microscopy (STM) experiments.[5] For one layer the easy magnetization axis is a twofold in-plane axis.[6,7] When monolayer stripes[8,9] or islands[10,11] are deposited on the Fe atomic monolayer the magnetization of these stripes and islands is perpendicular to the surface. Their exposure to residual gas rotates the magnetization in-plane.[8,10] This absorption driven spin transition is accompanied by a change of the coupling between the stripes or the islands from antiferromagnetic to ferromagnetic.

For the second Fe layer the experimental situation is more complicated. Although it was also believed that the second Fe layer grows pseudomorphically,[9] Sander *et al.* showed that already at 1.2 ML for a temperature of 300 K, misfit dislocations are created[10] and STM experiments confirmed dislocations starting from a 1.4 Fe monolayer.[5] At 1.5 ML, the misfit dislocations in the second layer serve as nucleation centers for the third layer that grows simultaneously with the second layer.[5] Elmers and Gradmann showed that such a film presents perpendicular magnetic anisotropy.[9]

The interpretation of the magnetic anisotropy energy (MAE) is a difficult task because it involves a small change in the total energy of the order of μeV to meV at the most, and it was shown[12] that not only states in the vicinity of the Fermi surface contribute to the MAE, but states far away make an equally important contribution. In the case of films the calculation of the MAE is even a more difficult task due to the low dimensionality. The early phenomenological model of Néel[13] for analyzing the MAE of ultrathin films is still widely applied for interpreting experimental data. In 1988, Draaisma and de Longe described the MAE of one-element unsupported film making use of its structure but did not take into account physical effects like the interlayer interaction.[14] In the case of a monolayer of a $3d$ transition metal, Bruno used a perturbative theory to express the spin-orbit arising anisotropy energy.[15] But the problem of the effect of the substrate on the magnetic anisotropy energy of the supported films has not been thoroughly investigated. *Ab initio* calculations can help to understand the interplay between the phenomena that are responsible for the MAE. One example is the case of Fe films on top of Au(001), where Szunyogh *et al.* using a layer version of the Korringa-Kohn-Rostocker method in the muffin-tin approximation predicted the spin reorientation from perpendicular to in-plane when one Fe layer was added to the trilayer film.[16] This transition was explained as due to the competition between the magnetosurface and the shape anisotropy.

On the other hand, the dichroism-type spectroscopy became a powerful tool in the study of the magnetic properties of materials.[17,18] The x-ray absorption spectroscopy using polarized radiation probes element specific magnetic properties of alloys and compounds via the x-ray magnetic circular dichroism (XMCD) in conjunction with the sum rules.[19] The XMCD sum rules permit the determination of the spin and orbital moments from the integrated XMCD spectra. So, the XMCD can be used to probe the size of the magnetocrystalline anisotropy (MCA) via the determination of the orbital moment anisotropy. Indeed, Bruno formulated a relation that connects the orbital moment anisotropy to the MCA in the case of the $3d$ transition metals.[15] This approach becomes valid only for systems where there are no holes in the

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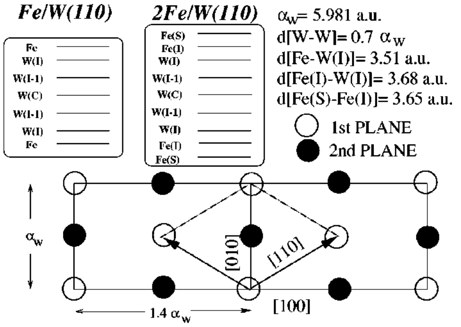

FIG. 1. Slab and two-dimensional structure of one and two layers of Fe on W(110) systems. a_W is the lattice constant for the bulk bcc W. Interlayer distances extracted by total energy calculations are presented.

spin-up band and the crystalline field parameter is much smaller than the spin-orbit coupling. van der Laan generalized this approach to the case where holes are also present in the spin-up band.[20] Nevertheless, a relation that strictly relates the MCA, or more generally the MAE, to the orbital moments is not yet developed, and so the discussion for low-dimension systems like films or surfaces is only valid at the qualitative level.

In this work we study the magnetic anisotropy energy of one, two, and three Fe atomic layers on top of a W(110) substrate as well as its connection to the interlayer distance and the anisotropy of the orbital magnetic moment and of the XMCD spectrum. To perform our calculations we have used the relativistic full-potential (FP) linear muffin-tin orbital (LMTO) method[21] in conjunction with the local spin-density approximation (LSDA).[22] In Sec. II we present the structural properties of Fe ultrathin films on W(110) and in Sec. III the magnetic anisotropy energy results. In Sec. IV the spin and orbital moments are discussed, and finally, we present the XMCD results.

II. STRUCTURAL PROPERTIES

Our study is based on a slab structure in a supercell geometry (see Fig. 1). We imposed symmetric slabs containing two Fe surfaces to avoid the creation of slab dipoles. We found that five W layers are enough for convergence, i.e., the density of central W(C) has the characteristics of bulk bcc W. Adding two more W layers increases the magnetic anisotropy energy by less than 3%, so five W layers are enough to describe the MAE. We have also converged the vacuum spacing between two slabs to avoid interslab interactions and found a value of 3.5 times and 5.5 times the bulk W lattice parameter for the monolayer and for the bilayer system, respectively. We have assumed that the second layer grows also pseudomorphically and relaxed only the positions of the Fe layers. These calculations showed that the distance between the Fe monolayer and the W substrate (d[Fe-W(I)]) should be reduced to 3.51 a.u. compared to the W-W interlayer distance (d[W-W]) of 4.23 a.u. to compensate for the two-dimensional expansion of the Fe lattice. The second Fe layer increased the d[Fe(I)-W(I)] interlayer distance. To compute the d[Fe(I)-W(I)] and d[Fe(S)-Fe(I)] interlayer distances we performed total energy calculations for different sets of these values and made a least-square fit to the total energy surface as a function of these two parameters. The minimum of the energy surface is obtained for d[Fe(S)-Fe(I)] = 3.65 a.u. and d[Fe(I)-W(I)] = 3.68 a.u., and corresponds to about 5% expansion compared to the equivalent d[Fe-W] interlayer distance in the monolayer system. This behavior is similar to that of 1 ML of Ag on top of the first Fe layer.[23] In the case of the trilayer film we did not perform total energy calculations because we should minimize the total energy with respect to three interlayer distances, which is time consuming. Instead, we assumed the first two Fe atomic layers as having the same positions as for the bilayer system and that the distance between the second Fe layer and the surface layer is the same as that between the two Fe layers in the bilayer film.

Several studies have been dedicated to the calculation of the structural properties of the monolayer Fe/W(110) system. Tober *et al.* used multiple scattering calculations to reproduce photoelectron patterns and found that d[Fe-W(I)] should be 3.91 a.u.[4] Batirev *et al.* used the full-potential linear augmented plane-waves method (FLAPW) in conjunction with the Carr-Parrinelo technique and found also a value considerably larger than ours of 3.92 a.u.[24] However, Hong *et al.* used a slab FLAPW method and found a value of 3.55 a.u.,[23] close to our value of 3.51 a.u. Recently Qian and Hübner used another version of the FLAPW and obtained a value of 3.73 a.u.[25] Albrecht *et al.* derived from low-energy electron diffraction experiment a value of 3.67 a.u.,[26] which is between our value and that of Qian and Hübner. The interlayer distance between the two first W layers, d[W(I)-W(I−1)], does not change much among different calculations. Tober *et al.* and Batirev *et al.* found values that are about 2.2% (Ref. 4) and 3.3% (Ref. 24) larger than the unrelaxed value of 4.23 a.u., respectively. However the value of Qian and Hübner is only 1.1% larger than the unrelaxed value, and for the next W interlayer distance, d[W(I-1)-W(C)], the expansion is less than 1%.[25]

For the bilayer system, only Qian and Hübner made a full relaxation and found that all the distances between W layers are expanded by less than 1.5% compared to bulk W.[25] The Fe interlayer distances were found to be different from our results. They obtained a larger interfacial distance d[Fe(I)-W(I)] of 3.83 a.u. compared to our value of 3.68 a.u. Their calculated Fe interlayer distance d[Fe(S)-Fe(I)] is considerably smaller than our value (3.34 a.u. compared to our value of 3.65 a.u.) and to the value in the bulk bcc Fe of 3.83 a.u.

III. MAGNETIC ANISOTROPY ENERGY

To be consistent with previous studies on the Fe/W(110) system, we separated the MAE into three different contributions: (i) the magnetosurface anisotropy (MSA) arising from the spin-orbit coupling that is different from the MCA due to the lower dimension of a film compared a bulk system, (ii) the magnetoelastic anisotropy (MLA) due to the change of the in-plane lattice parameter of Fe compared to the bulk value, and finally (iii) the shape anisotropy (SA) due to the many-body interactions between the spin magnetic moments.[27] The MSA and MLA are directly included in the electronic structure and their sum represents our calculated MAE, which is defined as the difference in total energy be-

TABLE I. Calculated spin magnetic moments for both Fe(I) and W(I) at the interface, the Fe(S) at the surface and the Fe(I+1) in the in-between layer for all the monolayer, the bilayer, and the trilayer systems, combined to the FLAPW (Ref. 25) and to the experimental results (Ref. 37). The difference between the two *ab initio* methods of the values for the Fe atoms that neighbor the W atoms is due to the different values of the Fe-W(I) distance obtained by the two methods.

	Fe/W(110)		2Fe/W(110)			3Fe/W(110)			
μ^{spin}	Fe	W(I)	Fe(S)	Fe(I)	W(I)	Fe(S)	Fe(I+1)	Fe(I)	W(I)
Our work	2.12	−0.08	2.82	2.07	−0.10	2.80	2.61	2.04	−0.09
FLAPW	2.54	−0.09	2.84	2.31	−0.10				
Experiment	2.53		2.77						

tween the perpendicular [001] and the in-plane [100] axis. This difference is converged up to 1 μRy with the number of **k** points inside the Brillouin-zone (BZ) (up to 2662 **k** points in the BZ were used). In our calculated anisotropy we have not included the SA. The calculation of this quantity can be either estimated using the relation $\mathrm{SA}=2\pi M_V^2$ in cgs units, where M_V is the mean magnetization density[28] that can be calculated from our spin magnetic moments, or directly calculate the anisotropy of the dipole interaction between the spin magnetic moments [as it has been already done in the case of Fe ultra thin films on top of a Au(001) substrate[16]]. The dipole interaction energy is the sum of the energy of each spin magnetic moment $\mu_{\mathbf{i}}$ in the field $\mathbf{h_i}$ created by all the other spin magnetic moments;[29] $E_{dipole}=\frac{1}{2}\Sigma_i \mu_{\mathbf{i}}\mathbf{h_i}$. We can rewrite this equation in Rydberg units as[30,31]

$$E_{dipole}=\frac{1}{c^2}\sum_{i\neq i'}\left[\frac{\mu_{\mathbf{i}}\cdot\mu_{\mathbf{i}'}}{|\mathbf{R_i}-\mathbf{R_{i'}}|^3}-3\frac{(\mu_{\mathbf{i}}\cdot\{\mathbf{R_i}-\mathbf{R_{i'}}\})(\mu_{i'}\cdot\{\mathbf{R_i}-\mathbf{R_{i'}}\})}{|\mathbf{R_i}-\mathbf{R_{i'}}|^5}\right], \qquad (1)$$

where $\mathbf{R_i}$ runs over the atomic positions and c, the speed of light, is 274.072 in atomic units.

For the monolayer system the easy axis is found to be the in-plane [100] axis, in agreement with the experimental results of Gradmann *et al.*[6,32] The total energy for this direction lies 3.63 meV lower than for the other in-plane axis [010] and 3.35 meV lower than for the perpendicular to the film [001] axis. Our value is considerably larger than the MAE of Elmers *et al.*[2] of 0.11 meV derived from the MAE value for thick films[9] using the value for one Fe layer capped by Ag.[33] We have also computed the MAE for the unrelaxed system (d[Fe-W(I)]$=4.03$ a.u.) and found a value of 4.87 meV which is about 1.52 meV larger than the relaxed value. The addition of one more layer of Fe changed the sign of the calculated MSA+MLA that now favors the [001] axis (the converged MSA+MLA value is −0.05 meV). For the trilayer film we found an in-plane magnetization axis and a calculated MSA+MLA value of 1.02 meV. Using Eq. (1) we obtained a value of 0.08 meV for the SA of the monolayer system. This value is close to the value of 0.11 meV obtained using the phenomenological expression presented above. The SA for the monolayer system is one order of magnitude smaller than MSA+MLA. For the bilayer system the calculated SA using Eq. (1) is 0.26 meV. This value is also close to the phenomenological SA value of 0.30 meV. The addition of the SA to the MSA+MLA changed the magnetization axis to the in-plane position for the bilayer system. Finally for the trilayer film the calculated SA is 0.43 meV and added to MSA+MLA gives a total MAE of 1.45 meV.

Experimentally, an analytical investigation has been carried out for the magnetic anisotropy of the bilayer system based on a phenomenological model.[34,35] But, as mentioned in the Introduction, the second layer is far from being pseudomorphic, so a description of the second Fe atomic layer similar to ours is insufficient to represent the experimental situation,[5] and, hence, both calculated MSA and MLA cannot be directly compared to the experimental results. The experimental SA is about 0.26 meV in agreement with our calculated value. The experimental MSA also favors the in-plane axis. But the total MAE for this system is −0.11 meV favoring an out-of-plane magnetization axis due to the huge MLA of −0.70 meV.[34–36]

IV. MAGNETIC MOMENTS

Our calculated spin moments are isotropic with respect to the magnetization axis. For the monolayer system the Fe spin moment is $2.12\mu_B$, close to the FLAPW value of Hong *et al.*[23] ($2.18\mu_B$). Qian and Hübner[25] FLAPW calculations, without the spin-orbit coupling, found a Fe spin moment of $2.54\mu_B$, considerably larger than both our values and that of Hong *et al.* Fe spin moments are different from the bulk Fe due to the strong hybridization effect between the Fe and the W atoms and the surface relaxation. It seems that the origin of the discrepancy between the different electronic structure methods is due to the small Fe-W(I) distance obtained in both our method and that of Hong *et al.* This assumption is strongly supported by the $2.59\mu_B$ value obtained by us and by the $2.56\mu_B$ value obtained by Hong *et al.* for the unrelaxed d[Fe-W(I)] distance of 4.03 a.u.[23] The experimental Fe spin moment measured by torsion oscillatory magnetometry, is $2.53\mu_B$ and is comparable to the value of Qian and Hübner, but the interlayer distance has not been measured.[37] The wolfram at the interface W(I) is antiferromagnetically coupled to Fe with a spin magnetic moment of $-0.08\mu_B$ (see Table I), in agreement with the Qian and Hübner W(I) spin moment of $-0.09\mu_B$.[25] Pizzagalli *et al.* have shown using a tight-binding method that Fe-Fe interaction favors the parallel alignment of the spin moments, while the Fe-W interaction favors an antiparallel alignment.[38]

The addition of a second layer of Fe has complex consequences on the magnetic properties of the Fe/W system. The surface Fe(S) atoms have now other Fe atoms as neighbors instead of W atoms and their spin magnetic moment increases to $2.82\mu_B$. The interface Fe atoms ([Fe(I)]) show a

TABLE II. Calculated spin and orbital magnetic moments for both Fe(I) and W(I) at the interface and Fe(S) at the surface for both the monolayer and the bilayer systems as a function of the magnetization axis. The spin moments show no anisotropy whereas the orbital moments do. The Fe spin moment of the monolayer system is closer to the bulk bcc value, while the spin magnetic moment of the Fe atom at the surface of the bilayer system approaches the atomic limit.

	Fe/W(110)		2Fe/W(110)		
	Fe	W(I)	Fe(S)	Fe(I)	W(I)
μ^{spin}	2.12	-0.08	2.82	2.07	-0.10
$\mu^{orbit}_{[100]}$	0.16	-0.04	0.08	0.09	-0.02
$\mu^{orbit}_{[001]}$	0.11	-0.02	0.09	0.07	-0.01

slightly reduced spin magnetic moment ($2.07\mu_B$) compared to Fe atoms in the monolayer system. The absolute value of the induced magnetic moment on W(I) is about the same ($\mu^{spin}_{W(I)}=-0.10\mu_B$). The calculations of Qian and Hübner[25] produced a spin magnetic moment of $2.84\mu_B$ for the Fe(S) similar to our value, and a $2.31\mu_B$ for the Fe(I) that is much larger than ours as was also the case for the Fe monolayer. Nevertheless the W at the interface has a spin moment of $-0.10\mu_B$, in agreement with ours. Experimentally only the spin moment for the Fe(S) atom is known and the value of $2.77\mu_B$ is in good agreement with our results.[37]

We have also calculated the spin magnetic moments for the trilayer system. Our calculated spin magnetic moments starting from the Fe layer at the interface are $2.04\mu_B$, $2.61\mu_B$, and $2.80\mu_B$, respectively. If we compare these moments to the calculated ones for the bilayer system we remark that the Fe layers at the interface and the surface have practically the same spin magnetic moments and they are not affected by the Fe layer in between. The spin moment of the W(I) at the interface depends on the hybridization with the first Fe atomic layer and so its value for the trilayer system of $-0.09\mu_B$ is very close to the values for the monolayer and the bilayer system of $-0.08\mu_B$ and $-0.10\mu_B$, respectively. For the trilayer unrelaxed system we did not calculate the orbital moments because they are very sensitive to the relaxation as shown in the monolayer and bilayer systems.

The orbital magnetic moments, contrary to the spin moments, present a strong anisotropy (see Table II). For 1 ML the in-plane orbital moments are much larger than these out of-plane. This anisotropy of the W(I) orbital moment is directly observed in the x-ray magnetic circular dichroism spectra (see next paragraph). Fe in the monolayer system and for the magnetization direction along the [100] axis has an orbital moment double than of the Fe(S) atom moment in the bilayer system and 78% larger than the Fe(I) atom. For the [001] axis the differences are not that pronounced. The Fe orbital moment in the monolayer system decreases by 31% when we pass from the [100] to the [001] axis, while for the bilayer system Fe(I) moment decreases by 22% and the Fe(S) moment increases just by 13%. This behavior of the orbital magnetic moments is due partially to the spin magnetic moment but the principal contribution comes from the crystal environment of each atom underlying the role of the W 5d orbitals. It is interesting to notice that the orbital moment anisotropy sign is the same for all the atoms [except the Fe(S) atom] in both systems but the magnetic anisotropy energy changes sign.

van der Laan[20] expanded Bruno's MAE relation[15] by taking into account the contribution of each spin-projected orbital magnetic moment via the spin-orbit coupling and the contribution of the spin asphericity due to spin flip excitations but neglected the dependence of the MAE on the film thickness and the difference in the magnetic behavior of each layer. These latter effects are important for Fe/W(110) and so van der Laan's expended Bruno's MAE relation remains inapplicable in the case of the Fe/W(110) system.

V. X-RAY MAGNETIC CIRCULAR DICHROISM

In the last part of this work we present the calculated XMCD spectra. The XMCD is defined as the difference in the absorption coefficients for left and right circular polarized x-ray radiation and for the $L_{2,3}$ edges it involves electronic excitations of $2p_{1/2}$ and $2p_{3/2}$ core electrons primarily towards $3d$ conduction states and to a lesser extend towards the $4s$ conduction states.[39] Using the sum rules[19] it is experimentally possible to probe element-specific magnetic properties of the d states. But their application especially for strongly itinerant electrons like the 5d of W and low-dimensional systems is strongly debated since the sum rules are derived from an atomic formalism.

The method for calculating the electron transition matrix elements and consequently the absorption coefficient has been presented elsewhere.[40] The theory based on LSDA is known to underestimate the integrated L_3/L_2 branching ratio but it reproduces the correct trends as a function of the magnetization direction.[41] For Fe, a Gaussian of 0.4 eV width and a Lorentzian of 1 eV width is used to broaden the spectra accounting for the experimental resolution and the core-hole lifetime broadening, respectively. In the case of W the $2p$ states are deeper in energy than for Fe and their lifetime is smaller; so to account for the core-hole lifetime broadening we use both a Gaussian and a Lorentzian of 1 eV width each. The screening of the core hole is more important for W than for Fe and so the influence of the redistribution of the electronic cloud (core-hole effect) on the final unoccupied states would be less important. There is no experimental XMCD spectra for the Fe ultrathin films on W(110).

Figure 2 shows the calculated XMCD spectra of the Fe and of W(I) atoms at the interface for the monolayer system. The energy difference in the position of the two peaks gives the spin-orbit splitting of the $2p$ core states, 12.5 eV for Fe and 1351.4 eV for W, and as a core-electron property it is insensitive to the crystal field. The most important feature of these spectra are the large anisotropy of the XMCD spectra of the W(I) atom reflecting its large orbital magnetic moment anisotropy. The integrated L_3/L_2 branching ratio is divided by more than 8 as we pass from the axis of the larger orbital magnetic moment, [100], to the [001] axis ($L_3/L_2=1.68$ for the [100] and 0.20 for the [001] axis), and both peaks change sign. This behavior can be explained qualitatively by means of the sum rules[19] by showing that the decrease of the orbital moment is related to the decrease of the integrated L_3/L_2 branching ratio explaining the anisotropy of the W's XMCD spectra. The site of Fe shows also an anisotropy in the XMCD spectra and the integrated L_3/L_2 branching ratio is

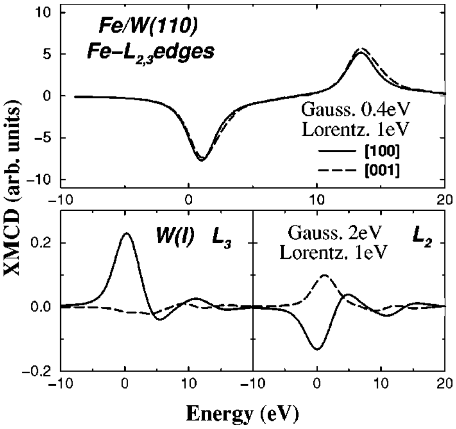

FIG. 2. X-ray magnetic circular dichroism at the $L_{2,3}$ edges of Fe and W(I) atom at the interface for the monolayer system. The integrated L_3/L_2 branching ratio follows the evolution of the orbital magnetic moments and decreases as we pass from the [100] to the [001] magnetization axis. The relative anisotropies are more important for the W(I) atom but the absolute values of the differences are one order magnitude larger for Fe.

about 1.43 for the [100] axis and 1.29 for the [001]. Although both Fe and W(I) atoms show roughly a similar percentage decrease of the orbital magnetic moment, the size of the XMCD anisotropy is quite different because of different (1) number of holes in the *d* band, (2) localization strength of the *d* orbitals, and (3) intensity of the core-hole effect.

Figure 3 shows the XMCD spectra for the bilayer system. The W(I) and the Fe(I) atoms present similar behavior as in the monolayer system. The integrated L_3/L_2 branching ratio follows the evolution of the orbital magnetic moments and for the Fe(I) atom changes from 1.32 for the [100] axis to 1.19 for the [001] axis and for the W(I) atom from 2.06 to 0.43. The W L_2 and L_3 peak intensities for both magnetization axes are more important than for the monolayer system reflecting the influence of the crystal environment on the XMCD. Although W in both systems presents a similar orbital anisotropy (see Table I) the XMCD anisotropy is more important for the monolayer system. The integrated L_3/L_2 branching ratio decreases by 79% in the bilayer system and by 88% in the monolayer system, while the orbital magnetic moment decreases by about 50% for both systems. The Fe atom at the surface shows practically no orbital moment anisotropy and this is also the case for the integrated L_3/L_2 branching ratio (1.16 for the [100] axis and 1.18 for the [001] axis), although $L_{2,3}$ peaks intensities change between the two magnetization axis.

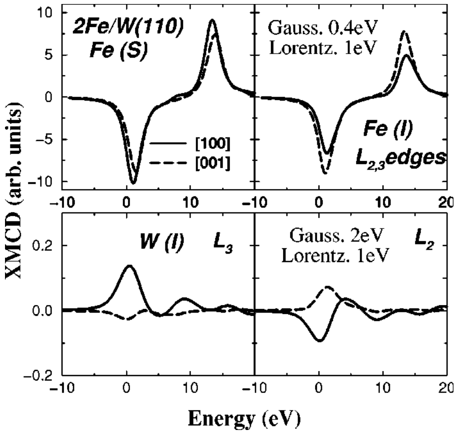

FIG. 3. X-ray magnetic circular dichroism at the $L_{2,3}$ edges of the Fe(S) atom at the surface and of the Fe(I) and W(I) atoms at the interface for the bilayer system. The atoms of Fe(I) and W(I) show a similar behavior than for the monolayer system. The Fe(S) presents a very small integrated L_3/L_2 branching ratio anisotropy reflecting its very small orbital magnetic anisotropy.

VI. CONCLUSION

In conclusion, we have conducted an *ab initio* full-potential linear muffin-tin orbital calculation of the magnetic anisotropy energy, and were able to produce the correct magnetization axis for one layer of Fe on W(110) substrate, and we predicted that for two and three Fe layers the magnetization axis should stay in-plane. Our calculations are not comparable to experiments because the second Fe layer is not growing pseudomorphically and at 1.5 Fe monolayers the third Fe atomic layer starts to grow simultaneously. The spin magnetic moment behavior can be explained in terms of the hybridization between the W 5d and the Fe 3d orbitals, and of the crystal environment of each atom. The spin moments for the Fe atoms that neighbor the W atoms depend on the distance between the layers. There is a large orbital anisotropy for all the atoms and especially for the W atom at the interface. Finally, we showed that this anisotropy is directly connected to that of the x-ray magnetic circular dichroism spectra.

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[1] M. Przybylski and U. Gradmann, Phys. Rev. Lett. **59**, 1152 (1987).

[2] H. J. Elmers, J. Hauschild, H. Höche, U. Gradmann, H. Bethge, and U. Köhler, Phys. Rev. Lett. **73**, 898 (1994).

[3] U. Gradmann and G. Waller, Surf. Sci. **116**, 539 (1982).

[4] E. D. Tober, R. X. Ynzunza, F. J. Palomares, Z. Wang, Z. Hussain, M. A. Van Hove, and C. S. Fadley, Phys. Rev. Lett. **79**, 2085 (1997).

[5] C. Jensen, K. Reshöft, and U. Köhler, Appl. Phys. A: Mater. Sci. Process. **62**, 217 (1996).

[6] U. Gradmann, J. Korecki, and G. Waller, Appl. Phys. A: Solids Surf. **39**, 101 (1986).

[7] H. J. Elmers, J. Hauschild, and U. Gradmann, Phys. Rev. B **54**, 15 224 (1996).

[8] H. J. Elmers, J. Hauschild, and U. Gradmann, Phys. Rev. B **59**, 3688 (1999).

[9] H. J. Elmers and U. Gradmann, Appl. Phys. A: Solids Surf. **51**, 255 (1990).

[10] D. Sander, R. Skomski, C. Schmidthals, A. Enders, and J. Kirschner, Phys. Rev. Lett. **77**, 2566 (1996).

[11] H. Dürkop, H. J. Elmers, and U. Gradmann, J. Magn. Magn. Mater. **172**, L1 (1997).

[12] G. H. O. Daalderop, P. J. Kelly, and M. F. H. Schuurmans, Phys. Rev. Lett. **71**, 2165 (1993).

[13] L. Néel, J. Phys. Radium **15**, 225 (1954).

[14] H. J. G. Draaisma and W. J. M. de Longe, J. Appl. Phys. **64**, 3610 (1988).

[15] P. Bruno, Phys. Rev. B **39**, 865 (1989).

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

[17] *Core Level Spectroscopies for Magnetic Phenomena: Theory and Experiment*, edited by P. S. Bagus, G. Pacchioni, and F. Parmigiani (Plenum, New York, 1995).

[18] *Spin-Orbit Influenced Spectroscopies of Magnetic Solids*, edited by H. Ebert and G. Schütz, Lecture Notes in Physics, Vol. 466 (Springer-Verlag, Heidelberg, 1996).

[19] For atoms: B. T. Thole, P. Carra, F. Sette, and G. van der Laan, Phys. Rev. Lett. **68**, 1943 (1992); P. Carra, B. T. Thole, M. Altarelli, and X. Wang, *ibid.* **70**, 694 (1993); G. van der Laan, Phys. Rev. B **57**, 112 (1998). For solids: A. Ankudinov and J. J. Rehr, *ibid.* **51**, 1282 (1995); G. Y. Guo, *ibid.* **57**, 10 295 (1998).

[20] G. van der Laan, J. Phys.: Condens. Matter **10**, 3239 (1998).

[21] J. M. Wills and B. R. Cooper, Phys. Rev. B **36**, 3809 (1987); M. Alouani and J. M. Wills, *ibid.* **54**, 2480 (1996).

[22] U. von Barth and L. Hedin, J. Phys. C **5**, 1629 (1972).

[23] S. C. Hong, A. J. Freeman, and C. L. Fu, Phys. Rev. B **38**, 12 156 (1988).

[24] I. G. Batirev, W. Hergert, P. Rennert, V. S. Stepanyuk, T. Ogushi, A. A. Katsnelson, J. A. Leiro, and K. H. Lee, Solid State Commun. **417**, 151 (1998).

[25] X. Qian and W. Hübner, Phys. Rev. B **60**, 16 192 (1999).

[26] M. Albrecht, U. Gradmann, Th. Reinert, and L. Fritsche, Solid State Commun. **78**, 671 (1991).

[27] H. J. F. Jansen, Phys. Rev. B **38**, 8022 (1988).

[28] P. Bruno, *Physical Origins and Theoretical Models of Magnetic Anisotropy* (Ferienkurse des Forschungszentrum Jülich, Jülich, 1993).

[29] A. Aharoni, *Introduction to the Theory of Ferromagnetism* (Oxford Science Publications, Oxford, 1998).

[30] B. R. A. Nijboer and F. W. De Wette, Physica **23**, 309 (1957); F. S. Ham and B. Segall, Phys. Rev. **124**, 1786 (1961); B. R. A. Nijboer and F. W. De Wette, Physica **24**, 422 (1958).

[31] G. H. O. Daalderop, P. J. Kelly, and M. F. H. Schuurmans, Phys. Rev. B **41**, 11 919 (1990).

[32] Notice that in the experimental papers the [110] axis is chosen as normal to the substrate, keeping the notation for the bulk W. These notations are different from ours, where the normal to the substrate is the [001], our [100] in-plane axis corresponds to the $[1\bar{1}0]$, and our [010] in-plane axis corresponds to the [001] axis in the experimental papers.

[33] U. Gradmann, M. Przybylski, H. J. Elmers, and G. Liu, Appl. Phys. A: Solids Surf. **49**, 563 (1989).

[34] N. Weber, K. Wagner, H. J. Elmers, J. Hauschild, and U. Gradmann, Phys. Rev. B **55**, 14 121 (1997).

[35] H. Fritzsche, H. J. Elmers, and U. Gradmann, J. Magn. Magn. Mater. **135**, 343 (1994).

[36] D. Sander, A. Enders, and J. Kirschner, J. Magn. Magn. Mater. **200**, 439 (1999).

[37] U. Gradmann, in *Handbook of Magnetic Materials*, edited by K. H. J. Buschow (North-Holland, Amsterdam, 1993), Vol. 7, Chap 1.

[38] L. Pizzagalli, D. Stoeffler, and F. Gautier, J. Magn. Magn. Mater. **154**, 213 (1996).

[39] M. Alouani, J. M. Wills, and J. W. Wilkins, Phys. Rev. B **57**, 9502 (1998); H. Ebert, Rep. Prog. Phys. **59**, 1665 (1996).

[40] I. Galanakis, S. Ostanin, M. Alouani, H. Dreyssé, and J. M. Wills, Phys. Rev. B **61**, 4093 (2000).

[41] W. Grange, I. Galanakis, M. Alouani, M. Maret, J.-P. Kappler, and A. Rogalev, Phys. Rev. B **62**, 1157 (2000).