Structural, electronic, and magnetic properties of clean and Ag-covered Fe monolayers on W(110)

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The structural, electronic, and magnetic properties of magnetic Fe transition-metal atoms as an overlayer on a nonmagnetic transition metal, W(110), and the effects of a Ag covering on the magnetism of Fe/W(110), are determined by means of the highly precise self-consistent all-electron full-potential linearized-augmented-plane-wave method based on the local-spin-density approximation. The interlayer spacings of Fe-W and Ag-Fe are determined from total-energy calculations. We find that the Fe atoms are relaxed downward (compared to the average of the Fe—Fe and W—W bulk bond lengths) by 9.5% and 4.0% for clean and Ag-covered Fe/W(110), respectively. We find that the hybridization of the W and Fe *d* bands plays an important role in determining the magnetism of the Fe/W(110) systems. The magnetic moment ($2.18\mu_B$) and the magnitude of the Fermi-contact hyperfine field (-148 kG) of the Fe in relaxed Fe/W(110) are greatly reduced compared to those of the unrelaxed Fe/W(110) (by $0.38\mu_B$ and 46 kG, respectively). The Ag covering increases the magnitude of the Fermi-contact term of the Fe by 29 kG by encouraging the indirect covalent spin polarization of the *s*-like electrons. If one includes estimates of the dipolar and unquenched orbital-angular-momentum contributions, then our calculated values of the hyperfine field are found to be in remarkable agreement with recent conversion-electron Mössbauer-spectroscopy experimental values.

I. INTRODUCTION

Experimental and theoretical studies on surface-interface magnetism have been exciting subjects since the early experimental reports of magnetically "dead" layers[1,2] for ferromagnetic transition-metal surfaces. A driving force in the study of the electronic structure and magnetism of transition-metal surfaces is the need to understand the role of surface and interface states and how the reduced coordination and symmetry lead to important property differences with respect to bulk systems.

A number of theoretical studies[3–6] on magnetic transition-metal surfaces have predicted interesting results including the enhancement of their surface magnetic moments with respect to their bulk values by 20–300 %. Thus, the effects of a surface on magnetism are fairly important. Particularly significant to the present study are the predicted enhancements of the Fe(001) and Fe(110) surface magnetic moments by[3] 35% and[6] 20%, respectively, but a sizable *decrease* in the magnitude of the total (negative) contact hyperfine field, H_c. Apparently, this reduction in H_c arises because the change in the direct (now positive) contribution from the conduction electrons exceeds the enhanced negative contribution (due to the enhanced magnetic moment) from the core electrons via core polarization.[7]

But beyond the study of surfaces, recent progress in the fabrication and property modification of artificial materials (thin films, overlayers, sandwiches, and modulated structures) has stimulated theoretical and computational efforts on these materials as well. To examine the possibility of 2D magnetism, a number of theoretical investigations for magnetic transition metals (Fe, Ni, Cr, V) as overlayers on noble metals (Ag, Au, Cu) (Refs. 8–13) have been reported. Here too, strongly enhanced magnetic moments were predicted. Thus, for example, giant moments ($3.70\mu_B$ and $3.5\mu_B$) were predicted for a ferromagnetic (FM) and antiferromagnetic (AFM) Cr monolayer on Au(001) along with a sizable magnetic moment ($0.14\mu_B$) induced onto neighboring Au atoms in the FM case; the magnetic moment of an Fe monolayer on Ag(001) (Refs. 10 and 11) was calculated to be very close to that of the clean Fe(001) surface,[3] indicating a lack of interaction with the substrate. (Note that in this case there is a close matching of the Fe and Ag lattice constants.)

Recent experiments have called attention to the case of a magnetic transition metal on a nonmagnetic transition metal [i.e., Fe/W(110)], and the possible effects on the electronic and magnetic properties expected from hybridization between the differing *d* bands of the overlayer and the substrate. Remarkably, recent low-energy electron diffraction (LEED) experiments showed that even though there is a large misfit (9.4%) in their lattice constants, Fe atoms grow pseudomorphically on W(110), i.e., with the same lattice parameter as the substrate.[14] Both spin- and angle-resolved photoemission spectroscopy (SPARPES) (Ref. 15) and conversion-electron Mössbauer-spectroscopy (CEMS) (Ref. 16) have been performed to understand the magnetism of Fe overlayers on W(110).

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SPARPES (Ref. 15) found a 20% enhancement of the total magnetic moment for bilayer coverage but a 50% reduction for monolayer coverage from a measurement at room temperature. However, CEMS (Ref. 16) observed that the Curie temperature for the clean Fe monolayer on W(110) is 210 K and so could not confirm the ferromagnetism at room temperature. Furthermore, CEMS experiments showed other very interesting results: a drastic reduction (in magnitude) of the magnetic hyperfine field (to -100 kG) for an Fe monolayer on W(110) compared to that (-340 kG) in bulk Fe in spite of both having almost the same magnetic moment. Previously,[17] we investigated the magnetism of unrelaxed Fe overlayers on W(110) and found the contact magnetic hyperfine field to be -194 kG, i.e., much higher than the CEMS value.

In this paper, we investigate the origin of the observed drastic reduction of the magnetic hyperfine field by means of a theoretical study of the electronic and magnetic properties of a relaxed Fe monolayer on W(110) and a relaxed Ag layer on Fe/W(110) using the highly precise full-potential linearized-augmented-plane-wave (FLAPW) (Ref. 18) method within the local-spin-density (LSD) approximation.[19,20] In Sec. II, the calculational method and theoretical approach are described briefly. Our calculated results (magnetic-moment, hyperfine field, and single-particle spectra) are presented in Sec. III; the effect of hybridization and the effect of negative pressure on the electronic and magnetic properties are discussed by comparing them with the theoretical results for clean Fe(110).[6] A comparison of these predictions to experimental results for Fe overlayers on W(110) includes a discussion of the effects of temperature. A summary and conclusions are given in the final section.

II. METHODOLOGY

To investigate the properties of the clean and Ag-covered Fe monolayers on W(110), we approximate this system as a single slab consisting of five layers of W(110) plus a monolayer of Fe (and Ag for the Ag-covered case) on each side. The two-dimensional lattice parameter and the W-W interatomic distance are taken to be those of bulk W. The interlayer spacings of Ag-Fe and Fe-W are determined from total-energy calculations.

The Kohn-Sham equations for this single slab are solved self-consistently using the FLAPW method.[18] In this method, no shape approximations are made to the potential or the charge density in solving Poisson's equation.[21] All the matrix elements for a general potential are rigorously taken into account in all parts of space. The lattice harmonics with angular momenta up to $l=8$ are employed to expand the charge density and potential and to construct wave functions inside the muffin-tin (MT) spheres. For the spin-polarized studies we employ the explicit form of von Barth and Hedin for the exchange-correlation potential.[22]

The core electrons are treated fully relativistically, whereas the valence electrons are treated semirelativistically,[23] i.e., keeping all the other relativistic terms in the Hamiltonian except spin-orbit coupling. About 2×280 and 2×350 basis functions for the clean and Ag-covered Fe on W(110) are used for each of the 18 **k** points in the irreducible wedge of the two-dimensional Brillouin zone, respectively. The covergence of these calculations is better than 3×10^{-4} $e/(\text{a.u.})^3$ rms difference in the total charge and spin densities.

III. RESULTS

A. Structural properties: Total-energy studies

In our previous study[17] of the unrelaxed Fe/W(110) we found the importance of the hybridization of Fe and W bands in determining the magnetism of the Fe atoms. Hence, before discussing the electronic structure and magnetism, we need to determine the Fe-W interlayer spacings of the clean Fe/W(110) and the Ag-covered Fe/W(110). The solid circles in Fig. 1 show the calculated total-energy difference as a function of the Fe-W interlayer spacing for the clean Fe/W(110). The data points are fitted to a parabola (solid line). For the clean Fe/W(110), we find that the total energy has its minimum at an Fe-W interlayer spacing of 3.55 a.u., which corresponds to a 9.5% downward relaxation compared to the unrelaxed Fe-W distance (defined as the average of the Fe—Fe and W—W bond lengths in their bulk). A low-energy electron diffraction experiment reported that clean Fe(110) does not show any surface relaxation.[24] Since it is known that more open structures suffer more relaxation,[25] this large relaxation in Fe/W(110) is probably due to the expanded two-dimensional lattice constant coming from the 9.4% misfit between Fe and W.

The direct comparison of a theoretical value with that of an experiment may not be possible for a clean Fe surface because Fe is such a good getter and CEMS experiments need very long counting times. Hence, a more reliable comparison with the CEMS results we need to investigate the case of Ag-covered Fe/W(110). Thus, we have

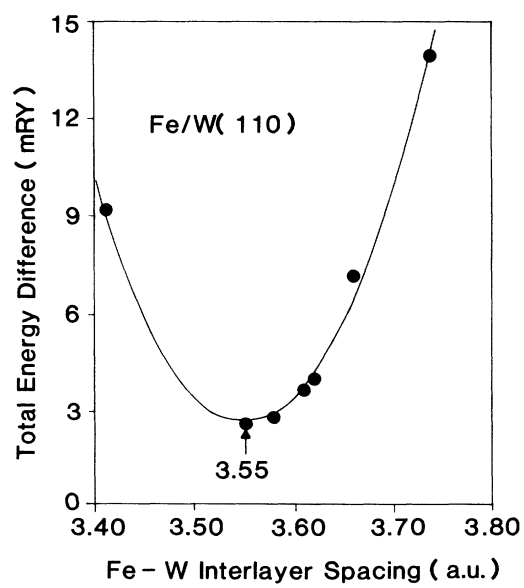

FIG. 1. Total-energy difference for the Fe/W(110) as a function of the Fe-W interlayer spacing. The arrow denotes the total-energy minimum.

two interlayer spacings (Ag-Fe and Fe-W) which affect the magnetism of the Fe. Here it is expected that the two interlayer spacings are quite independent of each other since different earlier studies[3,9,26–27] demonstrated short-range metallic screening for the charge density. For example, the amount of relaxation of the subsurface layer in W(001) (Ref. 26) and NiAl(110) (Ref. 27) is not affected by the amount of relaxation of the surface layer. Hence, we determine these two interlayer spacings at their total-energy minima by the following steps: First, we calculate the total energy of the Ag-covered Fe/W(110) as a function of the Fe-W interlayer spacing, while keeping the Ag-Fe interlayer spacing at a certain value [9% downward relaxed—almost the same value of the Fe relaxation in Fe/W(110)]. After finding a minimum total energy for the variation of the Fe-W interlayer spacing, we change the Ag-Fe interlayer spacing to obtain a stable structure of the Ag-covered Fe/W(110) while keeping the Fe-W interlayer spacing at the value which corresponds to the minimum total energy in the previous step.

Through these steps, we find a 4% downward relaxation for both of the Fe-W and Ag-Fe interlayer spacings (here again an unrelaxed Ag-Fe interatomic distance is defined to be the average of the Fe—Fe and Ag—Ag bond lengths in their bulk). The solid circles in Fig. 2 represent our calculated total-energy difference of the Ag-covered Fe/W(110) as a function of the Fe-W interlayer spacing. Here again, our calculated values are fitted to a parabola from which we find that the Fe-W interlayer spacing at equilibrium is 3.77 a.u. (corresponding to a 4% downward relaxation) which represents a much reduced relaxation compared to clean Fe/W(110). Since surface relaxation comes from the discontinuity of charge density at the surface, the Ag covering partially cures the discontinuity and imposes the bulk boundary conditions so as to reduce the amount of the relaxation.

B. Charge density and spin density

First, we discuss charge and spin densities which are fundamentally important quantities in LDS; these usually give insights for understanding the formation of the surface and interface. Figures 3 and 4 show contour maps of the charge and spin densities in the upper half of the slab for the relaxed clean and Ag-covered Fe/W(110), in units of 10^{-3} $e/(\text{a.u.})^3$ and 10^{-4} $e/(\text{a.u.})^3$, respectively.

We can see from the charge-density contour maps (cf Fig. 3) that electrons in the surface atoms (Fe or Ag) spill out into the vacuum to screen the abruptness of the surface and to lower their kinetic energy. The Ag covering discourages the spillout of the Fe electrons and so makes the charge configuration of Fe atoms in the Ag-covered Fe/W(110) more bulklike compared to that of clean Fe/W(110). The W atoms just one layer below the interface show almost the same charge configuration for both systems. Further, as compared by an angular-momentum decomposition of electrons within the MT spheres, the charge configuration of the subinterface W atoms is almost the same as that of the W atom in the center layer. This indicates that the screening length for charge density is very short, i.e., on the order of one atomic layer. As in other metals, interface effects on electronic properties are therefore confined only to interface atoms, and our slab model should be good enough to describe the properties of Fe overlayers on W(110).

Now, the work function has a direct physical significance in LSD and is determined in a delicate way by the spillout of electrons into vacuum. Thus, a study of the work function may also give some information about the surface formation indirectly. The calculated work functions for the clean and Ag-covered Fe/W (110) are 4.46 and 4.93 eV, respectively, whereas the W(110) surface shows a somewhat higher work function (5.30 eV).

The spin density [cf. Fig. 4(a)] of relaxed Fe/W(110) swells out into vacuum and shows a different shape from

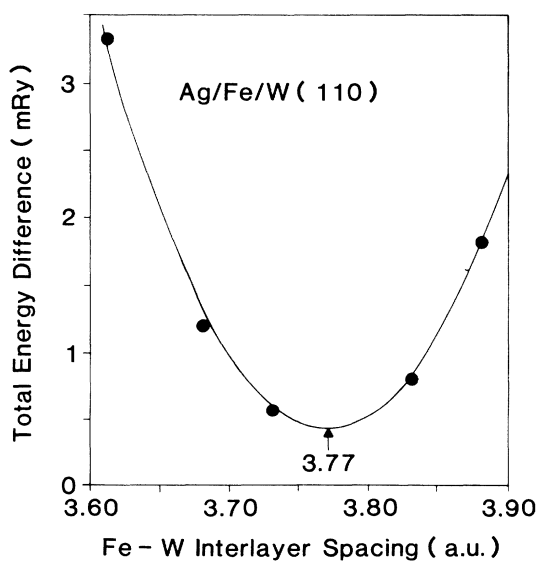

FIG. 2. Total-energy difference for the Ag-covered Fe/W(110) as a function of the Fe-W interlayer spacing. The arrow denotes the total-energy minimum.

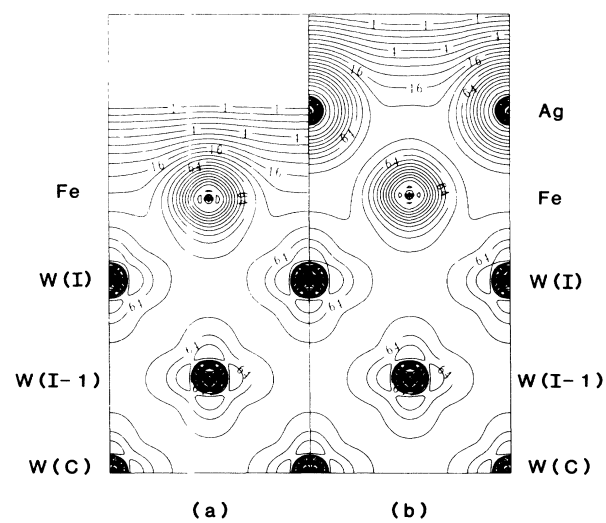

FIG. 3. Valence charge-density contour map for (a) Fe/W(110) and (b) Ag-covered Fe/W(110) on the (001) plane perpendicular to the surface in units of 10^{-3} $e/(\text{a.u.})^3$. Each contour line differs by a factor of $\sqrt{2}$.

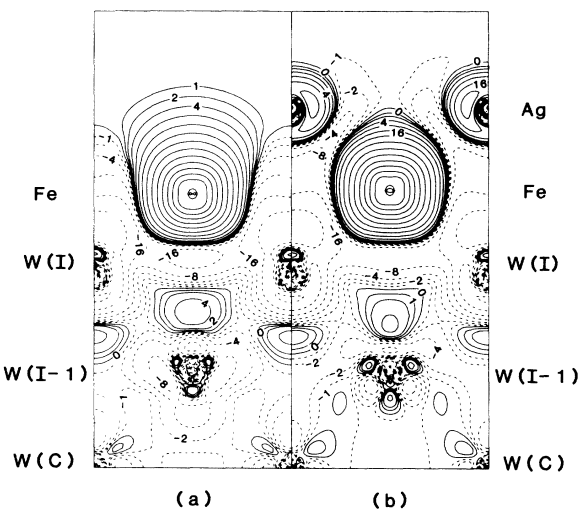

FIG. 4. Spin-density contour map for (a) Fe/W(110) and (b) the Ag-covered Fe/W(110) on the (001) plane perpendicular to the surface in units of 10^{-4} $e/(\text{a.u.})^3$. Each contour line differs by a factor of 2.

that of bulk Fe. As shown in Fig. 4(b), the Ag covering reduces the swellout spin density of clean Fe/W(110) by suppressing the d_{z^2} component of the spin density. However, the spin density of the Fe atoms still retains a surface feature by now swelling partially. The interface W layer is negatively polarized with a measurable magnetic moment of $-0.1\mu_B$, while the Ag layer is positively polarized with a relatively small magnetic moment of $0.02\mu_B$.

C. Magnetic moment and magnetic hyperfine field

The results for the relaxed clean and Ag-covered Fe/W(110) and the unrelaxed Fe/W(110), presented in Table I, indicate that the W(110) substrate, unlike the effect of noble-metal substrates,[9–11] reduces greatly the magnetic moments [$2.18\mu_B$ and $2.17\mu_B$ for the relaxed clean Fe/W(110) and Ag-covered Fe/W(110), respectively] compared to that ($2.98\mu_B$) of a free monolayer of Fe(110) with the same two-dimensional lattice constant as that of Fe/W(110) and that ($2.65\mu_B$) of the Fe(110) surface layer. By contrast, the Fe monolayer on noble-metal substrates retains almost the same magnetic moment as the unsupported Fe monolayer. Hence, the reduction of magnetic moment of Fe on the W substrate implies that the hybridization between the Fe d and W d bands plays an important role in determining the Fe magnetism. This hybridization also leads the magnetic moment of Fe in the relaxed Fe/W(110) to be greatly reduced compared to that ($2.56\mu_B$) of the unrelaxed Fe/W(110).

Kurzawa *et al.*[15] obtained a 50% reduction in the magnetic moment for monolayer Fe/W(110) at room temperature, using SPARPES, and pointed out that this reduction of magnetic moment is due to the lowered Curie temperature of this system. More recent experiments with CEMS (Ref. 16) did not observe any spontaneous magnetization for the clean Fe/W(110) at room temperature. However, their extrapolation to 0 K shows that the magnetic moment is almost the same as that of bulk Fe—a result that is consistent with our predictions.

The electronic spin density at the nucleus is the key quantity for the interpretation of the hyperfine-interaction measurements. It gives rise to the Fermi-contact hyperfine field (H_c) which is substantially larger than the contributions from any unquenched angular-momentum and dipolar fields. The calculated H_c values for the relaxed clean and Ag-covered Fe/W(110), and the unrelaxed Fe/W(110) and their decomposition into core- and conduction-electron (CE) contributions, are presented in Table I. As a result of their exchange interaction with the $3d$ moment, the core electrons which lie inside the $3d$ shell contribute a large negative value to H_c regardless of their environment.[7] As found for many bulk and surface systems, this contribution (cf. Table I) scales precisely with the magnetic moment. Hence, given the same magnetic moment, the contributions from core electrons for both relaxed, clean, and Ag-covered Fe/W(110) are almost the same as that of bulk Fe. However, the contribution from the $4s$ conduction electrons is strongly affected by their environment.[6,7,28,29]

In the bulk, the contribution from CE polarization is negative due to their indirect (covalent) polarization. The hyperfine fields of Fe atoms in the surface and interface layers, however, show positive contributions from the CE due to the direct polarization—similar to the case of free atoms. The large CE contribution for clean Fe/W(110) greatly reduces the magnitude of the total Fermi-contact term (-148 kG) compared to that (-350 kG) of bulklike Fe. The larger positive CE contribution from the Fe overlayers compared to that (-324 kG) of clean Fe(110) (Ref. 5) indicates that the s electrons in the overlayer Fe atoms are more atomiclike than those at the clean Fe(110) surface. The reasons for this are (1) the Fe—Fe bond length is larger than that of the clean Fe(110), and (2) the Fe $4s$ electrons hardly participate in the hybridization between Fe and W. Our calculations and the CEMS experiment confirm a striking demonstration that at surfaces and interfaces the total hyperfine

TABLE I. Theoretical layer-projected magnetic moments (in μ_B) and magnetic contact hyperfine fields (in kG) broken down into core and CE contributions for the relaxed Fe/W(110), Ag-covered Fe/W(110), and the unrelaxed Fe/W(110).

	Magnetic moment	Core	CE	Total	Core per M
Unrelaxed Fe/W(110)	2.56	−353	159	−194	−138
Relaxed Fe/W(110)	2.18	−306	158	−148	−141
Relaxed Ag/Fe/W(110)	2.17	−304	127	−177	−140

field is not proportional to the magnetic moment.

As shown in Table I, the Ag covering produces an additional negative indirect CE polarization of the *s*-like conduction electrons which when added to the positive CE polarization results in an enhancement of the magnitude of the total contact hyperfine field. The amount of enhancement (29 kG) is very consistent with the CEMS experimental value (20 kG).

Another important point is that the CE contribution does not change with the Fe-W interlayer spacing. As shown in Table I, the CE contribution of the relaxed Fe/W(110) is almost the same as that of the unrelaxed Fe/W(110) in spite of the large relaxation. Now the magnetic moment was found to decrease with the Fe-W interlayer spacing due to the strong hybridization between Fe 3*d* and W 5*d* bands. Hence, the total Fermi-contact term also varies linearly with the Fe-W interlayer spacing, as shown in Fig. 5. However, as expected, the Ag-Fe interlayer spacing does not significantly affect the magnetism of the Fe, including magnetic moment ($\Delta M = 0.1\mu_B$) and Fermi-contact term ($\Delta H_c = 4$ kG) in spite of the relatively large change (0.7 a.u.) of the interlayer spacing.

Although our calculated value of the Fermi-contact term is qualitatively consistent with the hyperfine field of the CEMS experiments, its magnitude is still higher than the experiment. Hence, we need to consider the remaining positive dipolar and unquenched angular-momentum contributions. Of course, these positive contributions would lead the theoretical magnetic hyperfine fields to be in better agreement with the experimental value. Furthermore, both terms are expected to be enhanced at a surface or at an interface. For convenience, the dipolar term is broken down into on-site and off-site contributions. The on-site contribution is found to be +6 kG. Now, the off-site contribution depends on the spin direction, which to our knowledge, is not known for Fe/W(110). If the spin direction is in the surface plane,[30] and using a crude classical point dipolar approximation, the off-site contribution is about +5 kG. By contrast, if the spin direction is perpendicular to the surface plane, then the same crude calculation gives −9 kG for the on-site contribution. Thus, the resulting total dipolar term is +11 or −3 kG, depending on the spin direction.

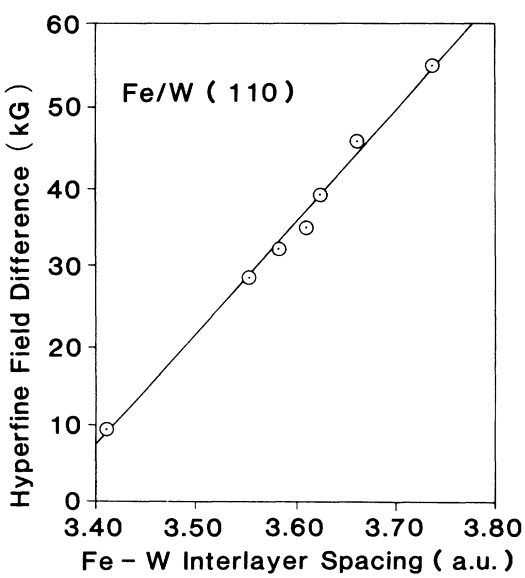

FIG. 5. Variation of the Fermi-contact term for Fe/W(110) as a function of the Fe-W interlayer spacing. The circles are our calculated data points which are fitted to a straight line.

The unquenched orbital-angular-momentum contribution (which arises from spin-orbit interaction) can be much larger than the dipolar contribution. Writing this as[7]

$$\Delta H_{\rm orb} = 125\,\Delta g \langle r^{-3} \rangle \text{ kG} ,$$

where $\langle r^{-3} \rangle$ is in a.u. and Δg is the g shift, then with[31] $\Delta g \simeq 0.09$ and[7] $\langle r^{-3} \rangle = 3.82$ a.u., $\Delta H_{\rm orb} = 44$ kG. Taken together with the dipolar contribution (+11 kG or −3 kG) and the contact value (−148 kG), this gives a total hyperfine field of −93 or −107 kG, which is in remarkable agreement with the CEMS experiment—especially in view of the crudeness of the various approximations.

D. Single-particle spectra

In order to understand the physical origin of the magnetic properties of clean Fe on W(110), we discuss the calculated energy-band structure and single-particle spectra. Figure 6 shows the layer-projected density of states (LDOS) for relaxed Fe/W(110). The left-hand (right-hand) side represents majority- (minority-) spin states. To establish the effects of (1) negative pressure due to the 9.4% misfit in the lattice constants, and (2) hybridization between the Fe 3*d* and W 5*d* bands, we also present in Fig. 7(a), 7(b), and 7(c) the LDOS of the unrelaxed Fe/W(110), the clean Fe(110) surface, and bulklike Fe, respectively.

The Fe LDOS in clean Fe/W(110) is a little bit different from that in clean Fe(110) due to the hybridization between the Fe 3*d* and W 5*d* bands. Compared to that of the unrelaxed Fe/W(110), the Fe LDOS of the relaxed Fe/W(110) is seen to become broader and more structured due to stronger interaction with the W substrate. The six major peaks of the Fe LDOS from majority-spin states between −3.5 and −1.0 eV below the Fermi energy (E_F) originate from the Fe atoms. The bandwidths of these peaks become narrower compared to that of the clean Fe(110) surface due to the expanded two-dimensional lattice constants. The peak at −4.3 eV below E_F and the peak just below E_F come from the hybridization with the W substrate. This interaction with the W substrate suppresses the surface states of the W(110) substrate.[32] For the minority-spin Fe LDOS, the interface states are seen clearly at −2.0 eV below E_F. For the minority-spin states, E_F lies above the valley separating bonding and antibonding states and indicates a reduction of the Fe magnetic moment for relaxed Fe/W(110). It is interesting to compare the location of E_F for Fe in different environments. In unrelaxed Fe/W(110) and bulk Fe [cf. Figs. 7(a) and 7(c)], the Fermi energy is pinned in the valley of the DOS and in the clean Fe(110) [cf. Fig. 7(b)] it lies below the valley.

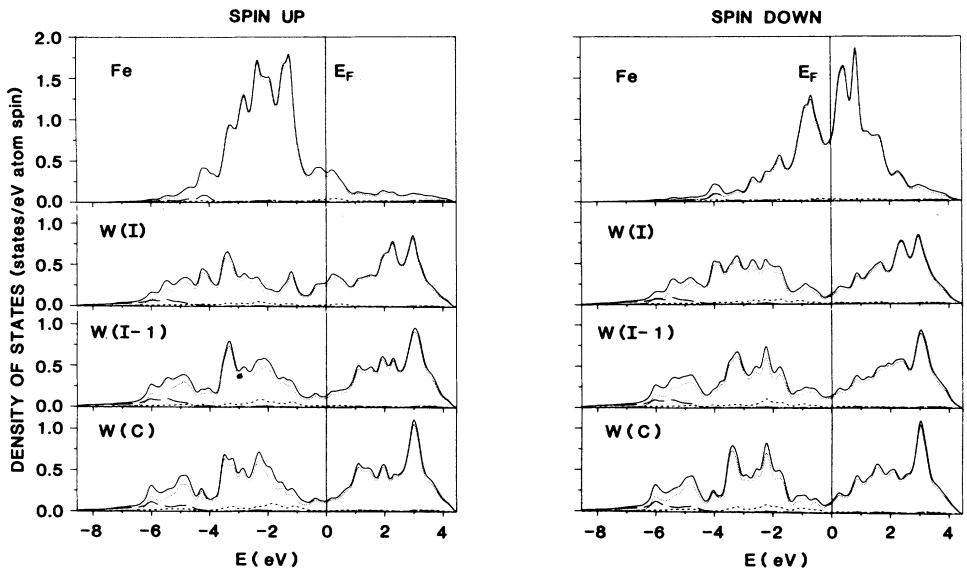

FIG. 6. Layer-projected partial density of states in units of states/eV spin for Fe/W(110). Dotted lines indicate d states and dashed lines represent s,p contributions.

The LDOS of Ag-covered Fe/W(110) is shown in Fig. 8. The Fe LDOS is now sharper compared to that of clean Fe/W(110), reflecting the weaker interaction with the W substrate coming from the reduced relaxation. The sharper peaks indicate also that the hybridization between the Fe and Ag atoms is relatively weak compared to the Fe-W hybridization. The LDOS for majority-spin states of the Ag layer shows some hybridization between the Fe and Ag atoms, while that for minority-spin states does not show any hybridization because of the nonoverlap between the Ag and Fe d bands.

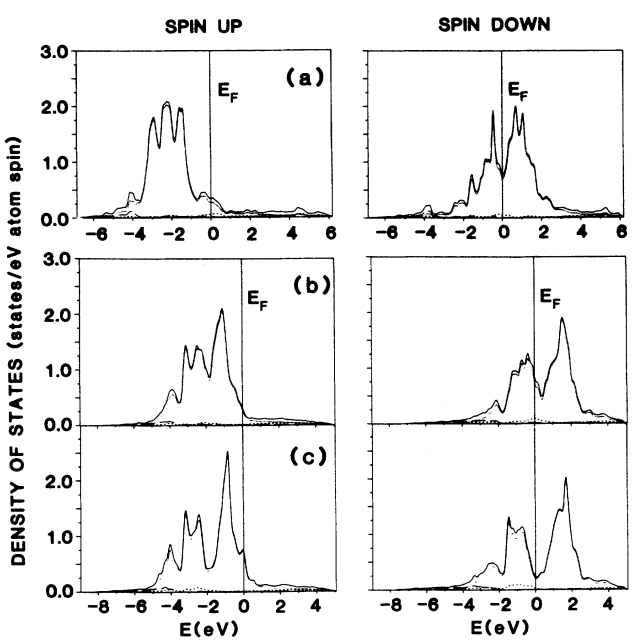

FIG. 7. Layer-projected partial density of states in units of states/eV spin for (a) unrelaxed Fe/W(110), (b) clean Fe(110), and (c) bulklike Fe. Dotted lines indicate d states and dashed lines represent s,p contributions.

Figures 9 and 10 show the band structure of relaxed clean and Ag-covered Fe/W(110). The bands are sorted for clarity according to their mirror-reflection symmetries: top (bottom) panels present the odd (even) parities with respect to the given symmetry line and the dashed (dotted) lines stand for the odd (even) symmetry with respect to z reflection. The left-hand (right-hand) panels represent majority- (minority-) spin states. Fe surface or interface states, defined as having their charge density localized by more than 50% in the Fe layer, are depicted by solid lines. The exchange splittings (ΔE_{ex}) of the Fe states are estimated to be the same value (about 1.9 eV) for both the relaxed clean and Ag-covered surfaces, which implies the Fe same magnetic moments for both systems, as shown in the preceding section. This value is much smaller than those of Fe/Cu(001) and Fe/Ag(001) where hybridization between overlayer and substrate is negligible. The Ag covering does not significantly change the band structure of the Fe states, which indicates again the weakness of the hybridization between Fe and Ag. The Ag covering makes the Fe bands less dispersive in the relaxed Ag-covered Fe/W(110) with respect to the relaxed Fe/W(110) due to the increased Fe-W interlayer spacing, as shown in Sec. III A. Further, the low-lying surface states at $\bar{\Gamma}_1$ (with binding energy of 5.2 and 4.6 eV for majority and minority spin, respectively) disappear when Ag covers Fe(110). We may conclude that these low-lying states are really attributable to the surface.

IV. SUMMARY AND CONCLUSIONS

We have discussed the structural, electronic, and magnetic properties of the clean and Ag-covered Fe/W(110) using the highly precise self-consistent all-electron

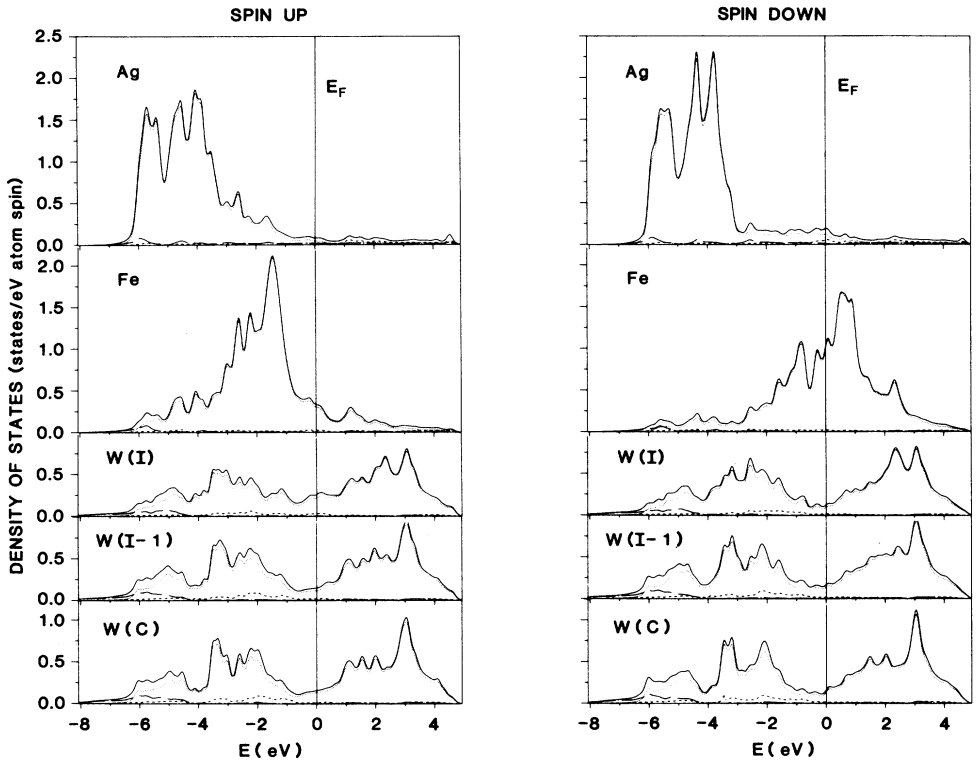

FIG. 8. Layer-projected partial density of states in units of states/eV spin for the Ag-covered Fe/W(110). Dotted lines indicate *d* states and dashed lines represent *s,p* contributions.

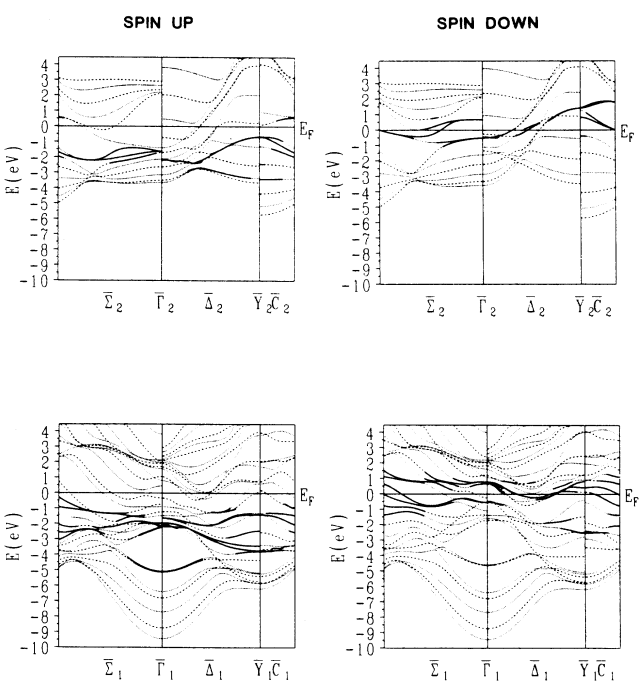

FIG. 9. Energy bands for relaxed Fe/W(110) or majority spin and minority spin along high-symmetry directions in the 2D Brillouin zone. Top and bottom panels show odd and even symmetries with respect to the given symmetry line. Dashed and dotted lines represent odd and even parities with respect to the central plane. Solid lines indicate surface states whose wave functions have more than 50% weight within the Fe layer.

FLAPW method based on the local-spin-density-functional approximation with a single-slab approach. The Fe atoms in Fe/W(110) are relaxed downward by 9.5% with respect to the Fe-W interlayer spacing determined as the average bond lengths of Fe—Fe and W—W in their bulk. This large relaxation and accompanying in-

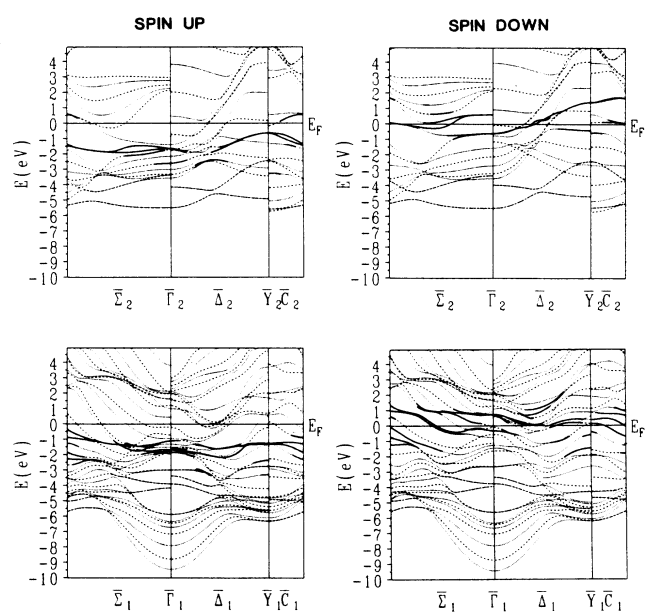

FIG. 10. Energy bands for relaxed Ag/Fe/W(110). Notations are the same as in Fig. 9.

crease of Fe $3d$ and W $5d$ hybridization causes the reduction of the Fe magnetic moment (to $2.18\mu_B$) and results in the decrease (in magnitude) of the contact magnetic hyperfine field (-148 kG) compared to those of unrelaxed Fe/W(110) by 46 kG. Together with the dipolar ($+11$ or -3 kG, depending on direction of the surface moment) and unquenched angular-momentum ($+44$ kG) terms, our calculated total hyperfine fields are in remarkable agreement with the CEMS result. The Ag covering leads the Fe atoms to be less relaxed, i.e., 4% downward. The resulting enhancement of magnetic moment from the reduced relaxation is compensated completely by the reduction in moment due to the proximity effect of the Ag layer. It is also found that the Ag-Fe interlayer spacing does not influence the magnetism of the Fe, significantly. Despite the same Fe magnetic moment, the Ag covering induces indirect covalent polarization of the s-like conduction electrons and so enhances the magnitude of the Fermi-contact term by 29 kG, which is consistent with the CEMS experimental value.

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