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Surface magnetism of Fe(001)

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Results of all-electron self-consistent semirelativistic full-potential linearized augmented-plane-wave local-density and local-spin-density studies are reported for a seven-layer Fe(001) thin film. The calculated work function for the ferromagnetic state is found to be in excellent agreement with experiment, whereas that calculated for the paramagnetic state is significantly worse (namely, 0.5 eV too large), indicating the importance of spin polarization on this electrostatic property. For both states, partial densities of states (projected by layer and by orbital angular momentum), surface states, and charge (and spin) densities are presented and their differences employed to discuss the origin of surface magnetism. No Friedel oscillation is found in the layer-by-layer charge density. The surface-layer magnetic moment is found to have been increased by $0.73\mu_B$ from the center layer to $2.98\mu_B$/atom; a very small Friedel oscillation is obtained for the spin density, which indicates possible size effects in this seven-layer film. Layer-by-layer Fermi contact hyperfine fields are presented: While the core-polarization contributions are proportional to the magnetic moment, the conduction-electron contribution shows a pronounced Friedel oscillation in the central layer and, significantly, a change of sign and increase in the magnitude for the surface-layer contribution. The hyperfine field at the nucleus of the center-layer atoms is found to be in excellent agreement with experiment. The net result for the surface-layer atoms is a predicted *decrease* in magnitude of the total Fermi contact hyperfine field despite the large increase of their magnetic moments. The relevance of this prediction to experiment is discussed.

I. INTRODUCTION

The surface magnetism of the 3*d* transition metals has become a subject of great theoretical and experimental interest in particular, because of possible changes of magnetism due to the existence of surface states and the different environment relative to bulk. The possibility of "magnetically dead layers"[1,2] at the surface of ferromagnetic Fe and Ni has invoked considerable discussion and has stimulated the development of theoretical methods for describing surface-electronic structures. A number of studies[3–8] by the finite-slab approximation to the semi-infinite solid show that electronic structures of the surface are well described by this finite-slab model. With the success of the local-spin-density functional theory in describing magnetism of bulk systems, it is of interest to assess predictions of surface magnetism obtained from *ab initio* self-consistent finite-slab calculations.

In earlier spin-polarized self-consistent studies of the magnetism of nine-layer Ni(001) (Ref. 9) and seven-layer Fe(001) (Ref. 10) films using the self-consistent-charge linear-combination of atomic orbitals discrete variational method (LCAO-DVM) approach, Wang and Freeman confirmed that the surface atoms still remain magnetic, which is consistent with recent precise experiments.[11–13] In the seven-layer Fe(001) calculation,[10] they found a large enhancement of the surface magnetic moment, a high surface density of states (DOS) in the valley of the bonding and antibonding (bulk) *d*-band peaks and a Fermi level which lies at the peak of the surface-state minority spin DOS. However, their layer-by-layer spin moments showed a strong Friedel-type oscillation from the surface to center layer of the film and the magnetic moment at the center layer was far from the bulk value, suggesting that a seven-layer model for Fe(001) surface was not thick enough to stabilize the oscillation. Because of this oscillation, it was difficult to understand the surface magnetism as a modification of the bulk magnetism and to understand the role of surface states in the enhancement of the surface magnetic moment.

To describe the surface electronic structure it is necessary to provide sufficient variational freedom. Insufficient variational freedom may cause unphysical oscillations in the "self-consistent" charge and spin densities, especially in the sensitive surface vacuum region. In this respect, the linearized augmented-plane-wave (LAPW) method applied to film systems[7] is known to be flexible enough to describe surface electronic structures because of the flexibility of the plane-wave basis. The recently developed full potential version (no shape approximation for the potential) of the film LAPW [FLAPW (Ref. 14)] is now established to be one of the most accurate electronic-structure methods for finite-slab calculations.

In this paper, we present results of an all-electron spin-

polarized semirelativistic study of a seven-layer Fe(001) system by the FLAPW method.[15] Self-consistent calculations were carried out for both the paramagnetic and ferromagnetic states of Fe(001) using the local (spin) density exchange-correlation scheme of von Barth—Hedin with the Hedin-Lundqvist potential[16] for the nonmagnetic case. In Sec. II, calculational models for both states are described; results are presented in Sec. III and finally discussions on surface magnetism are given in Sec. IV.

II. THEORETICAL AND/OR CALCULATIONAL MODEL

In an earlier theoretical study of surface states, surface magnetization, and electron-spin polarization of the Fe(001) surface, Wang and Freeman[10] used a LCAO thin-film method and found an enhancement of the surface magnetism and strong Friedel-type oscillations in the spin density. In this LCAO calculation a small variational basis and a superposition of spherical charges were used. Both computational restrictions can cloud the significance of the results, particularly for delicate quantities such as spin densities. We therefore undertook a reexamination of the electronic and magnetic surface properties and employed our highly accurate FLAPW method.

The FLAPW method[14] for thin films is the generalization of the film LAPW method[7] which takes nonspherical contributions to the potential in the muffin-tin (MT) sphere into consideration correctly by solving Poisson's equation for a general potential. In this approach no shape approximations are made to the charge density and the potential, and all matrix elements due to this full-potential are rigorously taken into account. All electrons are treated self-consistently, the core fully relativistically and the valence electrons semirelativistically. Therefore the FLAPW method allows not only the accurate calculation of valence spin densities but also an accurate treatment of the core polarization and hence makes possible the calculations of hyperfine fields at the nuclei.

In these calculations, the MT radius is $R_{\mathrm{MT}}=(\sqrt{3}/4)a$, where a is the bulk-lattice parameter ($a=5.4169$ a.u.), and the planar boundary of the film is set so as to touch the outermost MT spheres. The calculated results, however, do not depend on the internal division of space into MT, interstitial, and vacuum regions, since these are merely for mathematical and computational convenience in our full-potential method.[14] About 250 basis functions are used for each $\vec{k}$ point. Inside the MT spheres, lattice harmonics with $l \leq 8$ are employed to describe the charge and potential and are constructed from wave functions up to $l=8$. At first, a non-spin-polarized (paramagnetic state) seven-layer Fe(001) film with 16 $\vec{k}$ points in the irreducible $\frac{1}{8}$ wedge of the two-dimensional (2D) Brillouin zone was investigated self-consistently. After that, self-consistent spin-polarized calculations using 36 $\vec{k}$ points in the irreducible wedge were carried out starting with a small energy difference between both spin-state potentials. The convergence of both calculations is better than 5×10^{-4} electron/a.u.^{3} root-mean-square (rms) difference in the total charge density, which corresponds to a potential convergence of better than 5 mRy in the rms difference.

III. RESULTS

The final converged conduction-electron charge density, the central quantity in density-functional theory, is shown in Fig. 1 in the (110) plane. Several features are apparent here as they are in all film calculations for metals: Screening of the discontinuity introduced by the formation of a surface layer (S) is short ranged, with the charge density in the layer ($S-1$) just below the surface rapidly assuming the same contour values as those layers which are bulklike ($S-2$ and C). The charge density in these layers is well represented by a spherical (MT) approximation. The surface-layer charge density shows a marked change from that of the other layers; the outward flow of charge into the vacuum region serves to screen (heal) the surface discontinuity and to give rise to a dipole layer of charge which is responsible for creating the surface work function Φ. Indeed, as we shall see, the accurate prediction of Φ poses a severe test for the theory and provides a direct measure of the adequacy and accuracy of the film calculation.

Table I presents a comparison of the layer-by-layer electronic charge inside this MT for both the paramagnetic and ferromagnetic systems. The loss of charge inside the surface MT compared to the other layers is clearly seen. Spin polarization has not changed the electron count in the $S-2$ and C MT's but a small change (0.03 electron) exists at the S layer. This small change turns out to be

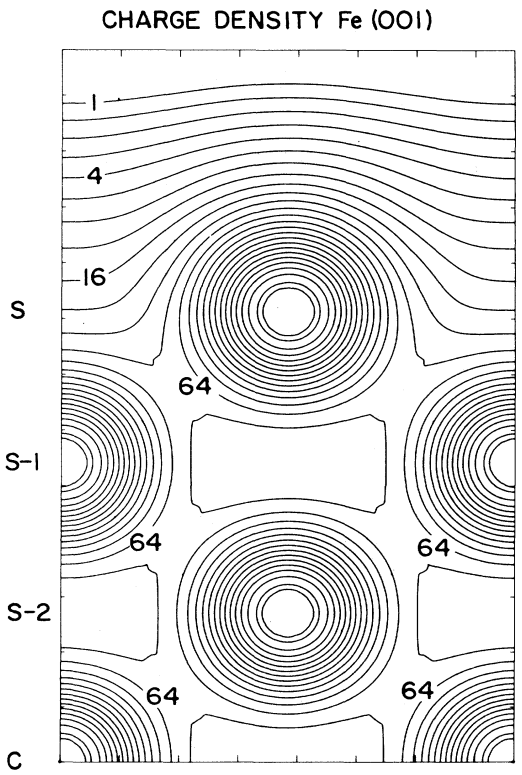

FIG. 1. Self-consistent conduction-electron charge-density map for the seven-layer Fe(001) film in units of 0.001 a.u. on the (110) plane. Each contour line differs by a factor of $\sqrt{2}$.

TABLE I. Theoretical work function, electronic charge, and magnetic moments for the seven-layer Fe(001) in the MT spheres in each layer from the surface (S) to the center (C) of the film. Valence charges are given in electrons and moments for the ferromagnetic state are given in μ_B.

	S	$S-1$	$S-2$	C	Work function (eV)
Paramagnetic charge	6.81	7.03	7.05	7.05	4.86
Ferromagnetic					
charge	6.78	7.05	7.05	7.05	4.29
spin	2.98	2.35	2.39	2.25	
Wang and Freeman	3.01[a]	1.69[a]	2.13[a]	1.89[a]	
Experiment				2.16[b]	4.31[c] 4.4[d]

[a]Reference 10.
[b]Reference 17.
[c]Reference 25.
[d]Reference 13.

significant for obtaining the correct work function for the system. Note that for the ferromagnetic case there is no Friedel oscillation in the charge. The self-consistent spin density ρ_s is shown for the (110) plane in Fig. 2. Unlike the charge density plotted in Fig. 1, the spin density is highly anisotropic and consists of both positive and negative regions. Away from the surface layer, the anisotropy (t_{2g}-to-e_g ratio) in the d-band ρ_s and the negative ρ_s between the atoms (in the bone-shaped structure) is consistent with that obtained by neutron magnetic scattering for bulk Fe. Unlike the case[9] of Ni(001), the eruption of ρ_s into the vacuum region is almost entirely positive and indicates a large increase in the magnetic moment at the surface. (This difference between Ni and Fe may be responsible for the reversal in sign of the magnetization inferred in spin-polarized tunneling and field-emission measurements.) The increase in magnetic moment at the surface ($2.98\mu_B$) over that of the center layer ($2.25\mu_B$) is seen in the layer-by-layer results shown in Table I, and the surface value is almost identical to the LCAO result given earlier by Wang and Freeman[10]—also given in Table I. However, unlike this earlier result, the magnetic moment in the C layer is close to the bulk value given by Wang and Callaway[17] and shows only a very small Friedel oscillation. Both the small increase in the moment at the center and the small Friedel oscillation indicate the presence of a size effect in this seven-layer film model used here. [Interestingly, a similar seven-layer FLAPW study[18] for Ni(001) gives the experimental bulk magnetic moment for the C layer and no Friedel oscillation in the moments at all.]

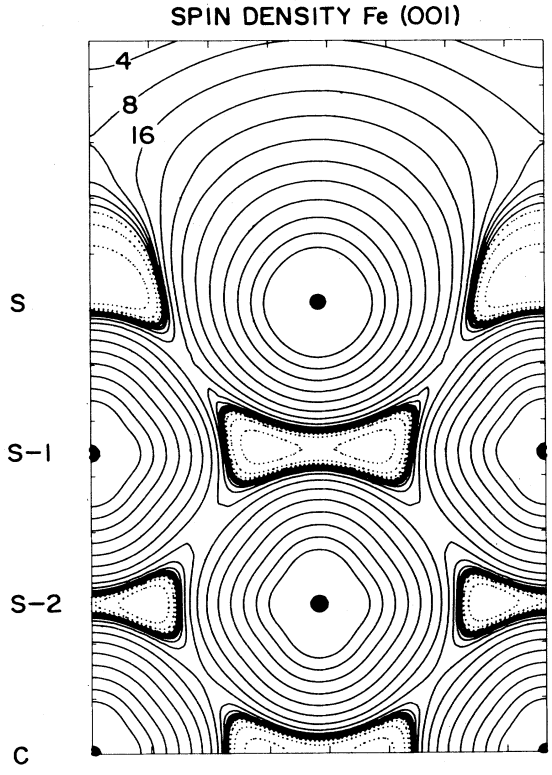

FIG. 2. Self-consistent spin-density map of seven-layer Fe(001) in units of 0.0001 a.u. on the (110) plane. Each contour line differs by a factor of 2. Dashed lines indicate negative spin density.

Decomposition of the majority- and minority-spin electrons inside the MT spheres by orbital angular momentum and by layer is given in Table II. Note the constancy of the number of s and p electrons in all the layers except for the S layer where the number of p electrons decreases due to their transfer into the vacuum region. The increase in magnetic moment at the surface is seen to be due to the increase (decrease) of the majority (minority) spin d electrons relative to their relatively constant values in the other layers.

Our calculated work function values for both the paramagnetic and ferromagnetic states are also given in Table I. We find that Φ for the ferromagnetic state (4.29 eV) is in very good agreement with experiment, whereas that calculated for the paramagnetic state (4.86 eV) is significantly worse. This error is much larger than the error ($\sim$0.1 eV) obtained with the FLAPW approach for other paramagnetic metals, and indicates for the first time the effect of magnetic order on a sensitive electrostatic quantity like Φ.

In order to understand the physical basis for these re-

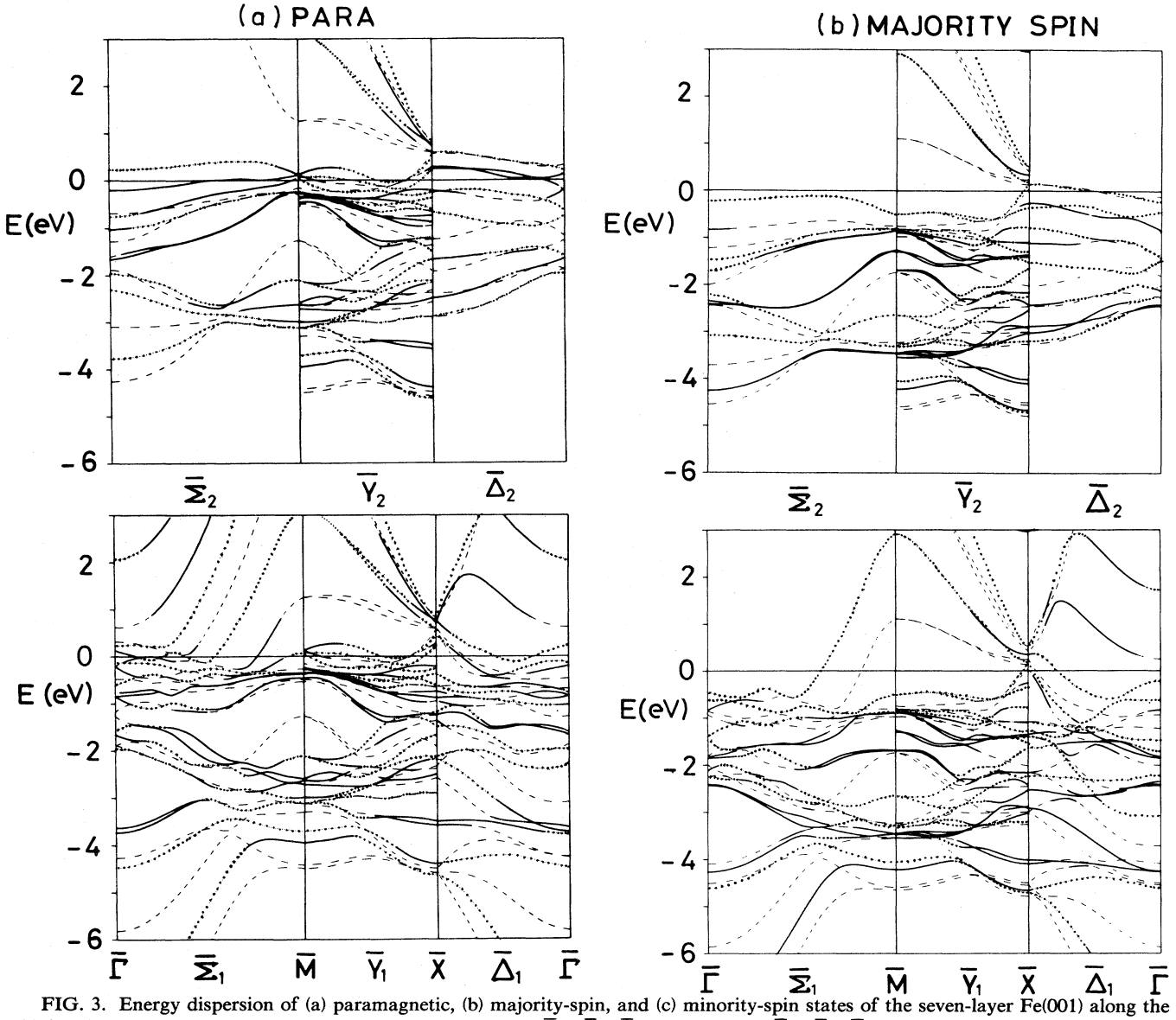

FIG. 3. Energy dispersion of (a) paramagnetic, (b) majority-spin, and (c) minority-spin states of the seven-layer Fe(001) along the high-symmetry directions in the 2D Brillouin zone. Top ($\bar{\Sigma}_2$–$\bar{Y}_2$–$\bar{\Delta}_2$) and bottom ($\bar{\Sigma}_1$–$\bar{Y}_1$–$\bar{\Delta}_1$) panels show odd and even symmetries with respect to the 2D rotational symmetry, respectively. — — — and ··· show odd and even symmetries with respect to the z-reflection symmetry, respectively. SS and SR with more than 70% localization in the first two surface layers are represented by solid lines. Fermi-energy level is set equal to zero.

sults, we now discuss the calculated energy-band structures and DOS. Figure 3 shows the calculated energy dispersions of the paramagnetic [Fig. 3(a)], majority-spin [Fig. 3(b)], and minority-spin states [Fig. 3(c)], broken down for clarity into their respective odd and even symmetries (with respect to 2D mirror planes). Surface energy bands are represented by solid curves defined as having their charge density localized by more than 70% in first

TABLE II. Decomposition of majority- and minority-spin electrons inside the MT spheres by l value and layer.

	Majority spin			Minority spin		
	s	p	d	s	p	d
S	0.21	0.13	4.54	0.19	0.12	1.60
$S-1$	0.20	0.19	4.31	0.21	0.22	1.92
$S-2$	0.20	0.20	4.32	0.21	0.22	1.90
C	0.20	0.20	4.25	0.21	0.23	1.97

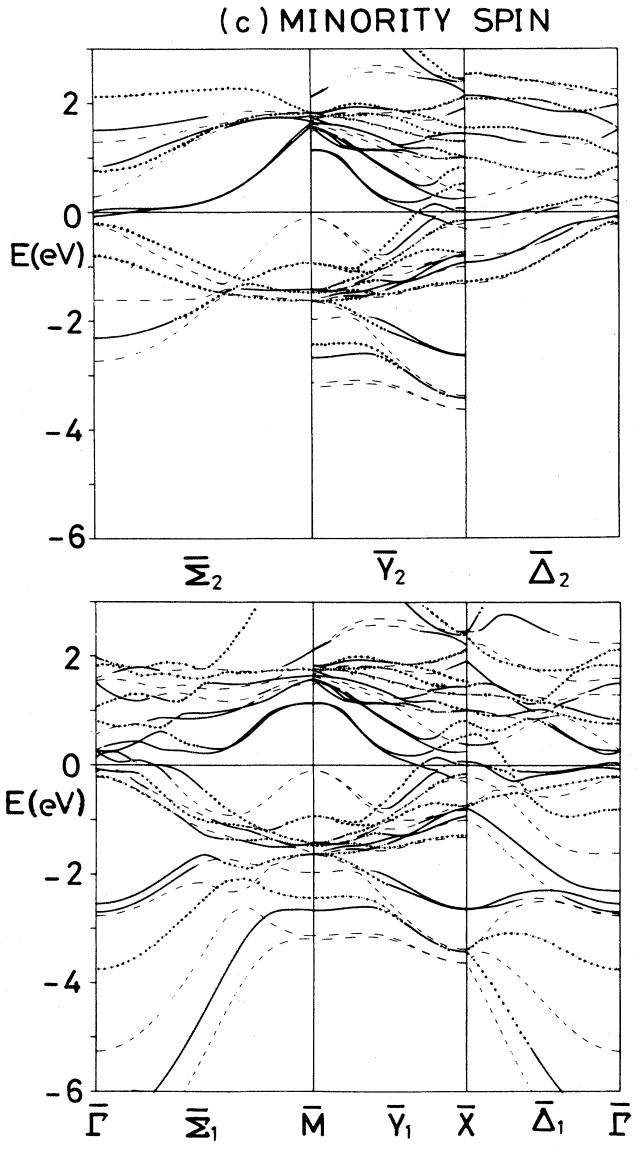

FIG. 3. (*Continued.*)

and second layers. We see a variety of surface states both above and below E_F. Recently, Turner *et al.*[13] reported energy dispersions of surface states in Fe(001) along $\bar{\Gamma}$ and $\bar{X}$ determined by angle-resolved photoemission spectra: They found that a surface state just below the Fermi energy exists in the entire region from $\bar{\Gamma}$ to $\bar{X}$ and a lower broad-band surface state has a dispersion from -2 to -3 eV. As seen from Fig. 3(c), the results of our calculation do show surface states of minority spin to lie just below the Fermi energy in the entire region from $\bar{\Gamma}$ to $\bar{X}$; those of majority spin have a dispersion from -0.88 to -0.25 eV, which may correspond to the double peaks or shoulder of the first peak below the Fermi energy seen in the photoemission data. In contrast, surface states in the paramagnetic calculation lie rather at a lower energy of -0.5 to -1 eV. In agreement with experiment, surface states between -2 and -3 eV are found in both majority- and minority-spin states. Note that such states are not found in the paramagnetic state around $\bar{\Gamma}$.

In Fig. 4, the l-decomposed partial DOS in the surface (S) and center (C) layer MT spheres are shown for both the paramagnetic and ferromagnetic films. The overall structures of both the majority- and minority-spin DOS are similar to the earlier LCAO results by Wang and Freeman[10] for the ferromagnetic state. Comparing the results for the S and C layers shows that surface states lie in the valley of the bonding and antibonding bulk peaks in both the paramagnetic and ferromagnetic cases. The Fermi level lies on the peak of the surface state of the minority-spin DOS.

In the paramagnetic state, the DOS at the Fermi level is very large; that for the surface layer is 1.5 times greater than that for the center layer. This high d DOS at the Fermi level suggests (in Stoner theory) that there will be a magnetic instability in bulk Fe and that there should be an enhancement of the magnetic moment at the surface relative to bulk. Note that the position of the surface-state peak relative to the bulklike d-band peaks is the same in both the paramagnetic and ferromagnetic cases and hence there is a rigid shift of the surface d states from the paramagnetic to the ferromagnetic structures. We can estimate the exchange splitting Δ, which varies over the d bands and also from the surface to center layer. At the center layer, Δ ranges from 1.36 eV (near the bottom of the d band) to 2.24 eV (near the topmost d band). These values are in agreement with those obtained in the bulk calculations by Callaway and Wang.[15] At the surface the splitting varies from 1.43 eV (near the bottom of the d band) to 2.39 eV (near the topmost of the d band). The exchange splitting of the surface layer is slightly larger (by about 6%) than that of the center layer; for the surface state Δ is 2.11 eV.

Finally, we have calculated the Fermi contact hyperfine interaction expected from our spin-polarized results. The dominant effect arises from the exchange-correlation polarization of the core electrons. Table III presents a layer-by-layer breakdown of the hyperfine field H_c into core and conduction-electron contributions. Several results stand out: (i) The total H_c for the C atoms (-336 kG) gives a total hyperfine field in excellent agreement with experiment if one includes a small (generally taken as 20 kG) positive contribution from unquenched orbital angular momentum. As emphasized by Kanamori,[19] aside from the early perturbative quasi-self-consistent result of Duff and Das,[20] no modern self-consistent local-spin-density calculation has yielded the correct hyperfine field for bulk Fe metal. The present full-potential result may therefore indicate the inadequacy of the shape approximations and/or basis sets used in these other studies. (ii) The contribution to H_c scales with the magnetic moment[21] (also shown for convenience in Table III) with a constant factor very close to that in the free atom. (iii) The conduction-electron contribution in the S layer is large and positive but negative for all the other layers. This causes the total H_c at the surface layer to be *reduced* in magnitude (-252 kG) compared to the bulk. This effect is all the more striking because the large increase in mag-

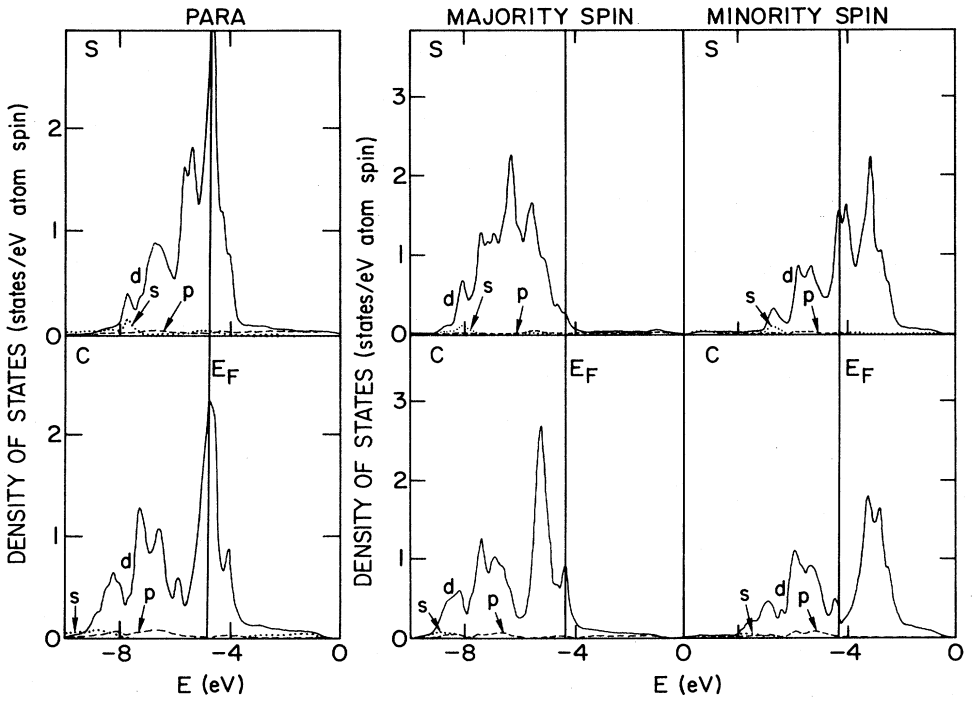

FIG. 4. Partial DOS (eV^{-1} $atom^{-1}$ $spin^{-1}$) decomposed by l value in the paramagnetic and ferromagnetic states of the seven-layer Fe(001) for the surface (S) and center (C) layers. They are smoothed by a Gaussian-broadening function of 0.075 eV FWHM.

netic moment and core contribution to H_c in the S layer would have indicated just the opposite. Apparently, as was seen also for the Pt(001) surface,[22] the expansion of the conduction electrons into the vacuum region causes them to be more free-electron-like and hence more easily polarized by the exchange-correlation potential.

Unfortunately, there are at present no hyperfine measurements available with which to compare these predictions for the clean Fe(001) surface. Since Fe is such a good getter, and since Mössbauer-effect measurements need long counting times, Walker and associates[23] have put an Ag overlayer on Fe to prevent oxidation. Since the Ag overlayer affects the Fe(001) surface magnetism,[24] the clean Fe(001) and the Ag/Fe(001) represent entirely different (but individually interesting) systems.

IV. DISCUSSION

From our seven-layer Fe(001) calculation, we can exclude the possibility of the enhanced surface magnetism resulting from a strong Friedel-oscillation mechanism of the spin moment. We can say that the enhancement of the magnetism occurs only at the surface layer. Figure 5 shows the difference, δD, between the surface and central layer DOS in the paramagnetic system. The lower (negative) peak comes from the bonding d-band peak and the higher (positive) peak comes from the surface states. We can understand this since the surface states are made up of bonding d orbitals from atoms which lose one-half of their nearest neighbors when at the surface. The main point will be that the energy of these surface states is not higher than that of the bulk antibonding bands. By using δD, we can calculate the difference magnetic moment, δM, between surface and center layers by assuming a rigid-band model of the paramagnetic DOS such as

$$\delta \mathrm{M}=\mu_B \int_{-\infty}^{E_F} [\delta D(E+\tfrac{1}{2}\Delta)-\delta D(E-\tfrac{1}{2}\Delta)]dE \ , \quad (1)$$

where E_F is the Fermi energy. In Fig. 6, values of δM vs E_F are plotted for several Δ's. Setting $E_F=4.86$ eV

TABLE III. Layer-by-layer hyperfine field and magnetic moment in the seven-layer Fe(001) film.

	Moment (μ_B)	Hyperfine field (kG) Core	Conduction electron	Total
S	2.98	−398	+143	−252
$S-1$	2.35	−306	−89	−395
$S-2$	2.39	−311	−16	−320
C	2.25	−291	−75	−366

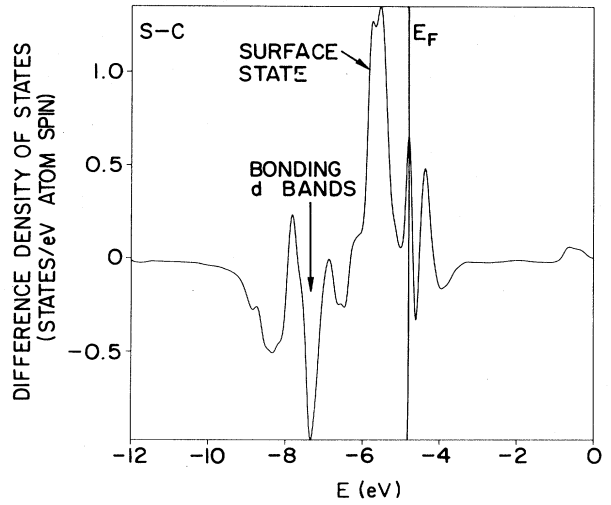

FIG. 5. Difference DOS δD between surface and center layers of the paramagnetic system.

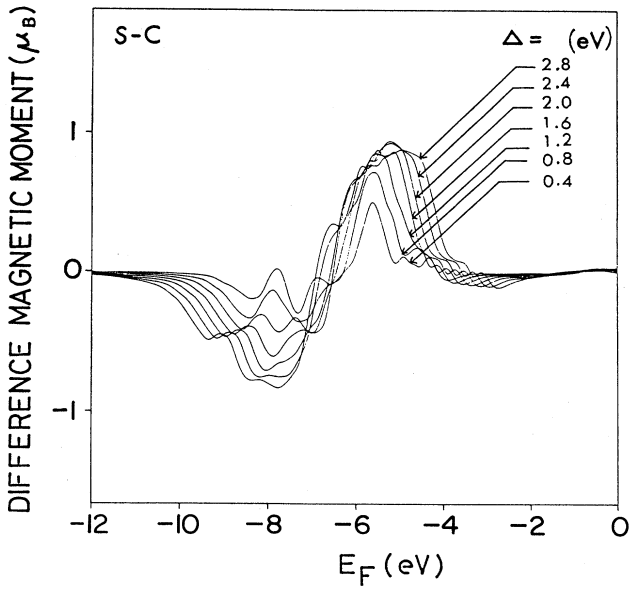

FIG. 6. Difference magnetic moment δM between surface and center layers; Δ is the exchange splitting, E_F is the Fermi energy, and δM is calculated by the rigid-band model by using Eq. (1).

(paramagnetic case) and $\Delta=2$ eV, δM becomes about $0.8\mu_B$, which is very close to the self-consistent result of $0.73\mu_B$. If we set $\Delta=1.7$ eV, δM becomes equal to $0.7\mu_B$. Thus, this model works quite well in providing an understanding of the enhancement of the surface magnetism obtained in the spin-polarized self-consistent calculation. It is easy to observe that the main contribution to the integral in Eq. (1) comes not from the bonding d-band peak, but rather from the surface-state peak because of the cancellation of the integrated values from the bonding d-band peak between $\delta D\,(E+\frac{1}{2}\Delta)$ and $\delta D\,(E-\frac{1}{2}\Delta)$ terms. Since the surface-state peak in Fig. 5 lies less than 1 eV $\approx\frac{1}{2}\Delta$ below the Fermi energy, the contribution from this surface-state peak in the minority term $\delta D\,(E-\frac{1}{2}\Delta)$ to δM is small, hence δM is determined mainly by the surface-state peak. As a result, the surface states are responsible for the enhancement of the surface magnetism. Figure 6 indicates this situation. Here we plot the difference in magnetic moment versus the location of E_F. To get the enhancement of the surface magnetism, the Fermi energy should be close to the surface-state peak (≈ -5.6 eV) in the case of small Δ so as not to be influenced by the surface-state peak of the minority term, $\delta D(E-\frac{1}{2}\Delta)$. In the case of large Δ, the enhancement of the magnetic moment occurs when the Fermi energy lies in the energy region from approximately -0.3Δ to 0.7Δ relative to the peak position of the surface state. It should be noted that a reduced moment at the surface is possible only in the restricted cases of the Fermi energy being in the middle of the bonding d-band peak and hence with E_F far below the surface-state peak.

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