Giant monolayer magnetization of Fe on MgO: A nearly ideal two-dimensional magnetic system

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(Received 30 July 1990)

Studies of the structural, electronic, and magnetic properties of a model 3*d* ferromagnetic metal-ceramic interface system Fe/MgO(001) by the full-potential linearized augmented-plane-wave total-energy method are reported. Surprisingly, the electronic and magnetic properties of a monolayer of Fe on MgO(001) substrate (magnetic moment $M=3.07\mu_B$) are remarkably close to that of a free-standing Fe monolayer (with a giant moment $M=3.10\mu_B$), as a result of the lack of electronic interaction between Fe and MgO. (The charge transfer at the Fe/MgO interface is less than 0.05 *e*/atom and so any direct chemical interaction between Fe and MgO is unlikely.) Thus, this system might be an ideal two-dimensional system for studying other phenomena such as magnetic anisotropy, phase transitions, and critical behavior. For two layers of Fe on MgO, i.e., 2Fe/MgO(001), the top layer Fe($M=2.96\mu_B$) shows features close to that of a free bcc Fe(001) surface ($M=2.96\mu_B$). Significantly, the magnetic moment of the Fe layer that interfaces the MgO substrate ($M=2.85\mu_B$) is also largely enhanced from the subsurface moment ($2.35\mu_B$) in bcc Fe(001), again indicating an extremely weak effect from the MgO substrate.

I. INTRODUCTION

Two-dimensional (2D) magnetism has been pursued with great intensity for the past decade, stimulated by newly developed precise theoretical approaches and sophisticated epitaxial and heteroepitaxial synthesis techniques. In the search for exotic phenomena expected in 2D, significant progress has already been made—particularly with 2D epitaxially grown monolayers—in studying enhanced magnetization, magnetic anisotropy, phase transitions, and critical behavior. Still, problems with the electronic and magnetic coupling of the overlayer to the substrate have introduced strong deviations from ideal 2D behavior. Simultaneously, epitaxial ferromagnetic thin films on various metallic substrates have been extensively studied in recent years because of their potential applications to electronics, high density recording devices, catalysis, etc. At 3*d* ferromagnetic transition metal (Fe, Co, and Ni) surfaces, novel features in their electronic and magnetic properties are conspicuous: enhanced magnetic moments at the surface from their bulk values, narrowed bandwidth of the surface layer density of states, and the existence of surface electronic states. The surface effect is usually limited to the topmost atomic layer for the non-close-packed surfaces—such as the (100) surface of cubic metals; the second atomic layer usually shows primarily bulklike features. A common technique to study monolayer magnetism is to epitaxially grow monolayer-range ferromagnetic thin films onto nonmagnetic metal substrates.

Generally, enhanced magnetic moments have been predicted for 3*d* transition metal surfaces and thin films compared with their bulk counterparts. A good example might be the Fe systems which have been intensively studied in recent years. Bulk bcc Fe has a magnetic moment of $\sim 2.2\mu_B$.[11] Enhancement of the magnetic moment is seen at the free surface of bcc Fe(001) ($M=2.98\mu_B$) because of the reduced symmetry and lower coordination number. Even larger magnetic moments can be achieved theoretically in free-standing monolayer Fe(001) ($M=\sim 3.1\mu_B$). Previous full-potential linearized augmented-plane-wave (FLAPW) computational studies of monolayer Fe on Ag(001) and Au(001) substrates [both Ag(001) and Au(001) closely match the bcc Fe lattice constant] show enhanced magnetic moments of Fe atoms ($2.97\mu_B$ in Fe/Ag and $2.98\mu_B$ in Fe/Au). These magnetic moments are very close to that of the free bcc Fe(001) surface, yet somewhat smaller than that of the free-standing Fe monolayer. The difference in results between overlayer Fe on a noble metal substrate and a free-standing Fe monolayer arises from the hybridization between the substrate and overlayer electronic states.

On the other hand, the behavior of magnetic ultrathin films on an insulating substrate has been much less researched. The experimental research on Fe/MgO is of interest from several perspectives. As early as 1972, Kanaji *et al.*[1] prepared epitaxial Fe(001) thin films on an MgO(001) substrate. The LEED pattern identified the orientations, $[001]_{Fe}\|[001]_{MgO}$ and $[100]_{Fe}\|[110]_{MgO}$. Their next work[2] showed that the Fe films grew epitaxially and monolayer by monolayer on the carefully cleaned MgO surface, and that the growth mode of the deposited film is affected by residual carbon contamination. Most recently,[3] their LEED and Auger electron spectroscopy (AES) results on Fe thin films deposited on a MgO(001) surface confirmed the layer-by-layer growth mode. Furthermore, the observations showed that (i) Fe films grow pseudomorphically and that the Fe atoms sit just above the oxygen ions for one monolayer average thickness, and (ii) the structure of an iron film is body-centered tetragonal (bct) in the early stage of growth, but it begins to change to the bcc structure at about 10 Å. Hubert

et al.[4] used transmission electron microscopy (TEM) techniques to study the microscopic structure of their evaporated Fe thin films on MgO. Further, as a result of heating, small particles of Fe were seen at ~350 °C, but disappeared above ~500 °C. It is also interesting to note the work of Nagao *et al.*,[5] who reported that iron films (a few atomic layers in thickness) grow epitaxially inside both (001) and (110) MgO films of about 25 nm thickness. Finally, Boudart *et al.*[6] reported a series of studies on the surface, catalytic, and magnetic properties of very small Fe particles (sizes down to at least ~1.5 nm) on MgO, primarily aimed at obtaining large surface areas for Fe catalysis.

The first *ab initio* all-electron theoretical studies on a metal/ceramic interface was reported in our previous work the Ag/MgO(001) system.[7] In Ag/MgO(001), the Ag atoms were found to prefer the sites above the substrate O atoms. Monolayer Ag adsorbed on MgO(001) shows metallic features with only a slight hybridization between the Ag *s,p* electron states and the interface O 2*s* states. In this work, we reported results of a model calculation of the Fe/MgO(001) interface, undertaken in hopes of gaining insights into the bonding mechanisms between these types of materials, their electronic structure, and most interestingly, the magnetic properties of this system.

II. METHODOLOGY AND COMPUTATIONAL METHODS

To study the structural, electronic, and magnetic properties of Fe/MgO, we applied the full-potential linearized augmented plane-wave (FLAPW) total-energy method[8] on systems containing one or two Fe monolayers adsorbed on the MgO(001) surface. In the FLAPW method for solving the local spin density functional (LSDF) equations,[9] no shape approximations are assumed when describing either the charge densities or the potential for the electronic system and highly precise all-electron total energies can be obtained. A fully relativistic Hamiltonian for the core electrons and a semirelativistic Hamiltonian (i.e., no spin-orbit interaction) for valence electrons are used throughout the self-consistent iterations. The von Barth and Hedin[10] form of the exchange-correlation potential is employed for spin-polarized calculations.

Two computational models were used: (i) monolayer Fe adsorbed on the MgO(001) surface, represented by a sandwich structure of one monolayer Fe placed on both sides of a five-layer MgO(001) single slab; and (ii) two Fe layers on MgO(001), represented by two layers of Fe placed on both sides of a five-layer MgO(001) single slab. The position of the monolayer Fe atoms on MgO(001) was determined by a total-energy analysis—described in Sec. III A. The Fe to MgO interface structure in 2Fe/MgO(001) was assumed to be the same as in 1Fe/MgO(001). For all atoms, spherical harmonics of angular momentum up to $l=8$ were used to construct the LAPW basis wave functions, charge densities, and potential within the muffin-tin (MT) spheres. The MT radii used for Fe, O, and Mg atoms were 2.2, 2.1, and 1.7 a.u., respectively. The Mg 1*s* and 2*s*, O 1*s*, and Fe 1*s*, 2*s*, 2*p*, 3*s*, and 3*p* electrons were treated as core electrons, and all the others were treated as valence electrons. The spin densities and magnetic moments were obtained from the spin-polarized calculations for the ferromagnetic phase of both 1Fe/MgO(001) and 2Fe/MgO(001).

For comparison of properties, reference calculations were also carried out on a clean five-layer MgO(001) single slab and a free-standing Fe monolayer using the same FLAPW computational procedures.

III. RESULTS AND DISCUSSION

A. Site preference and interlayer spacing of Fe on MgO(001)

To determine the interface structure between Fe and MgO(001), we studied two different positions for monolayer Fe on MgO(001), i.e., Fe above the O site and above the Mg site. The total-energy studies determined that Fe above the O atom site is the preferred position, similar to the results of the previous Ag/MgO(001) calculations.[7] The interlayer spacing between monolayer Fe and the MgO(001) substrate, 2.30 Å, was also determined by our total-energy calculations. [In the following, the properties of the Fe/MgO(001) system correspond to the case of the Fe above O site with this optimized interlayer spacing.] The same interface structure between Fe and MgO, i.e., the interface Fe atoms sitting at 2.30 Å above O sites, was assumed in our model calculations for 2Fe/MgO(001).

The site preference predicted by our calculations is consistent with the experimental findings by Urano and Kanaji,[3] namely, Fe atoms in monolayer range Fe thin films sit just above the oxygen atoms of the MgO(001) surface. The interlayer spacing found in this work, ~2.30 Å, is considerably larger than that reported by Urano and Kanaji (~2.0 Å) from their LEED *I-V* curve fitting results using dynamical calculations. It is very interesting to note the following in the work of Urano and Kanaji: (i) dynamical calculations show significant differences in LEED *I-V* curves for the three possible Fe sites considered (i.e., above O ion, above Mg ion, and bridge site), which provides a sound basis for their site determination of the Fe overlayer on MgO(001); (ii) their calculated LEED *I-V* curves for the Fe sites considered appear to be rather insensitive to the interlayer spacing between Fe and MgO, yet the experimental *I-V* curve (2 Å average overlayer thickness) retains only three major peaks and lacks the fine profile compared with the calculated curve—which leads us to question the accuracy of their determination of the Fe to MgO interlayer spacing. Note that the Fe-O distance is 2.14 Å in FeO and 2.10 Å (Fe*I*) in Fe_3O_4, respectively. Naturally, a larger Fe-O distance in Fe/MgO(001) (compared with both FeO and Fe_3O_4) should be anticipated, because the radius of an Fe atom is larger than that of an Fe^{2+} ion by 0.4 Å (or Fe^{3+} by 0.6 Å) in FeO (or Fe_3O_4).

B. Monolayer Fe on MgO(001)

1. *Charge and spin densities*

The charge density contour plot of ferromagnetic 1Fe/MgO(001) is shown in Fig. 1(a). As expected, the charge density of the MgO substrate remains primarily unchanged in comparison with clean MgO (shown in Ref. 7). The charge density contours for the O and Mg atoms have spherical shapes, and a small interface effect is seen at the interface O atoms. The Fe atom shows a surface-like charge distribution, i.e., with the charge smoothly extended into the vacuum region. The charge population of the atoms is listed in Table I. The overlayer Fe atom has a total charge of 6.31, which is equal to that of the free-standing Fe monolayer, in spite of the underlying MgO(001) substrate. Also interestingly, the MgO electron population in 1Fe/MgO(001) differs from that of the clean MgO(001) surface by only ~ 0.02 electron at the interface O atom, while the population of the other atoms remains almost unchanged. Thus, any strong direct interaction between Fe and MgO can be ruled out.

Shown in Fig. 1(b) is the spin density contour plot of ferromagnetic 1Fe/MgO(001) in the (100) plane. Large positive spin density is seen at the overlayer Fe atom, showing a *d*-like shape. Some negative spin density appears in the interstitial region between the overlayer Fe atoms (i.e., the region above the interface Mg atom). At the interface O atom, the positive net spin density has a *p*-like shape, indicating the slight influence of the magnetic Fe overlayer on the $2p$ electronic states of the interface O. The other atoms, i.e., all Mg atoms and the noninterface O atoms in the MgO(001) substrate, show almost no net spin density. The calculated magnetic moment, $3.07\mu_B$, is very close in value to that of a free-standing Fe monolayer ($3.10\mu_B$), and hence larger than that of the bcc Fe free surface value ($2.98\mu_B$),[11] or of Fe monolayers on noble metal surfaces[13] [$2.98\mu_B$ on Au and $2.97\mu_B$ on Ag(001)]. (The difference in magnetic moments resulting from the slightly different muffin-tin sphere radii utilized in these calculations is no larger than $0.05\mu_B$.)

TABLE I. Layer and *l*-projected muffin-tin charge population and magnetic moments (in μ_B) of O, Mg, and Fe in the calculated systems.

Atom	Layer		*s*	*p*	*d*	Total	Moment
			1Fe/MgO(001)				
Fe	Overlayer	↑	0.15	0.07	4.48	6.31	3.07
		↓	0.12	0.05	1.45		
O	Interface		1.84	4.60	0.02	6.47	0.03
	I-1		1.84	4.68	0.02	6.54	0.00
	Center		1.84	4.68	0.02	6.54	0.00
Mg	Interface		0.08	5.89	0.04	6.01	0.00
	I-1		0.08	5.91	0.05	6.04	0.00
	Center		0.08	5.90	0.05	6.03	0.00
			2Fe/MgO(001)				
Fe	Surface	↑	0.16	0.08	4.44	6.40	2.96
		↓	0.15	0.08	1.49		
Fe	$S-1$	↑	0.15	0.09	4.40	6.43	2.85
		↓	0.14	0.10	1.55		
O	Interface		1.84	4.61	0.02	6.45	0.03
	I-1		1.84	4.68	0.02	6.53	0.00
	Center		1.84	4.68	0.02	6.53	0.00
Mg	Interface		0.08	5.89	0.04	6.02	0.00
	I-1		0.08	5.91	0.05	6.04	0.00
	Center		0.08	5.90	0.05	6.04	0.00
			Clean five-layer MgO(001)				
O	Surface		1.83	4.59	0.02	6.44	
	$S-1$		1.84	4.67	0.02	6.53	
	Center		1.84	4.68	0.02	6.53	
Mg	Surface		0.08	5.90	0.04	6.02	
	$S-1$		0.08	5.91	0.05	6.04	
	Center		0.08	5.91	0.05	6.04	
			Free-standing Fe(001)				
Fe		↑	0.16	0.04	4.50	6.31	3.10
		↓	0.13	0.03	1.45		

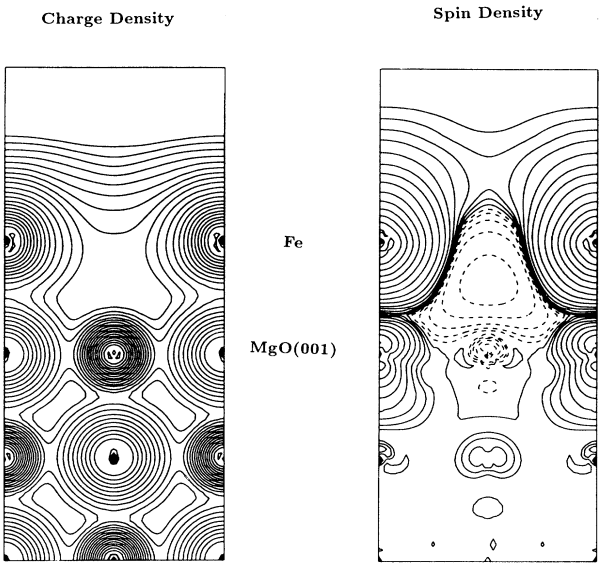

FIG. 1. (a) Charge and (b) spin density distributions for Fe/MgO(001) (Fe above O) plotted for the upper half of a single slab unit cell in the (100) plane. Numbers indicated are in units of (a) 0.001 e/a.u.^{3} and (b) 10^{-4} e/a.u.^{3}; subsequent contour lines by a factor of $\sqrt{2}$ in (a) and 2 in (b).

2. *Band structure and density of states*

Shown in Fig. 2 is the spin-polarized electronic band structure of 1Fe/MgO(001) along high symmetry directions. Solid lines indicate electronic states having more than 50% weight of the wave function within the Fe muffin-tin spheres. In the majority spin bands, the Fe 3d states appear in the energy range -4.2 to -1.8 eV below E_F, and are thus fully occupied. There is one s-p-like band crossing the Fermi energy. The top of the O 2p band appears at ~ -3.5 eV below E_F at the $\bar{\Gamma}$ point. There is a small overlap between O 2p and Fe 3d states in the vicinity of the $\bar{\Gamma}_1$ point which results in a small hybridization between these two bands. In the minority spin bands, the Fe 3d states are seen in the energy range from -0.8 eV below E_F to $+1.5$ eV above E_F. The bottom of an Fe s-p-like band appears to lie -3 eV below E_F at the $\bar{\Gamma}_1$ point. The substrate O 2p states remain the same as those seen in the majority spin bands. There is no overlap between the Fe and MgO minority spin bands.

Shown in Fig. 3 is the layer-projected density of states (DOS) for 1Fe/MgO(001) of both majority and minority spin directions. As for the free Fe atom, the majority spin states are fully occupied. The bandwidth of the Fe majority spin states is 1.8 eV, with the top of the band located 1.8 eV below the Femi energy. The Fe minority

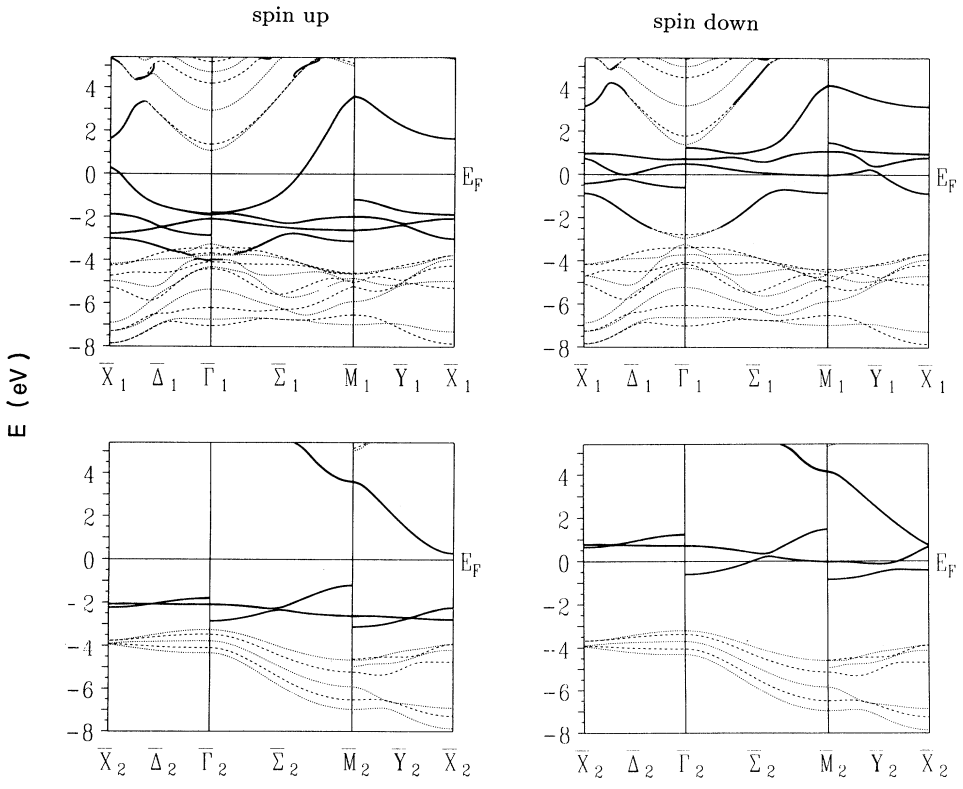

FIG. 2. Electronic band structure of 1Fe/MgO(001): (a) spin up and (b) spin down along high symmetry directions in the 2D Brillouin zone (BZ). Top and lower panels show odd and even symmetry, respectively, with respect to the 2D rotational symmetry. Dashed and dotted lines represent odd and even parity with respect to z reflection. Heavy solid lines indicate surface states identified as having more than 50% of their wave functions within the surface layer.

spin band is partially occupied and has a bandwidth of 2.2 eV. The exchange splitting of the Fe $3d$ bands is 2.8 eV. It is interesting to note that the minority spin Fe DOS has a sharp minimum around E_F.

C. 2Fe/MgO(001)

The charge density contour plot of 2Fe/MgO(001) in the (100) plane is shown in Fig. 4(a). The charge density

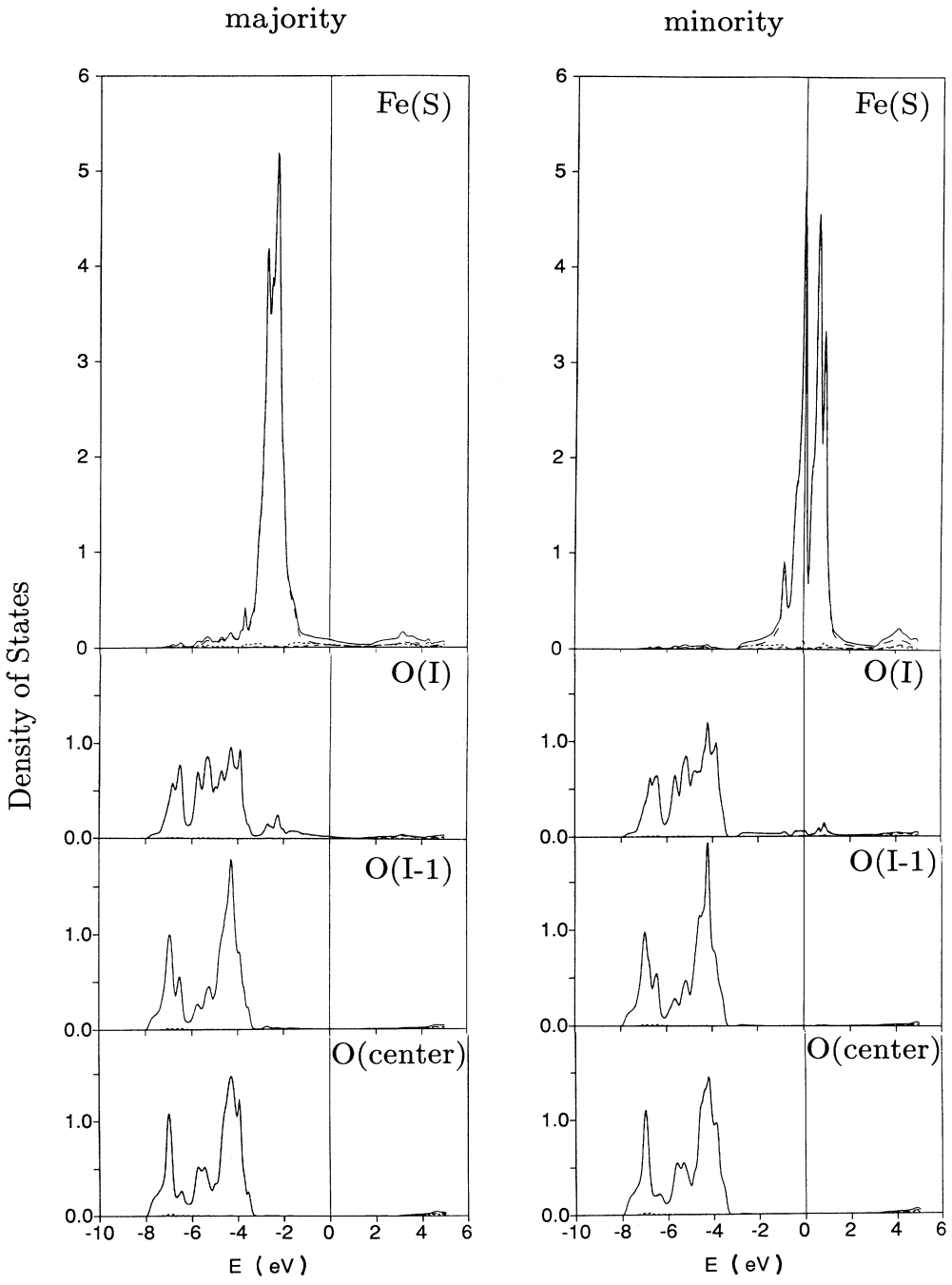

FIG. 3. The layer-projected partial density of states of the conduction electrons in units of states/eV atom for 1Fe/MgO(001) (Fe above O site).

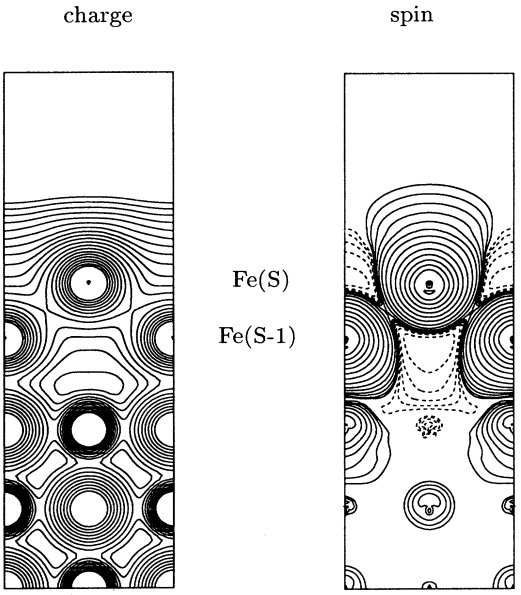

FIG. 4. (a) Charge and (b) spin density in the (100) plane of 2Fe/MgO(001)—as in Fig. 1.

shape of the MgO substrate in 2Fe/MgO is close to that seen in both 1Fe/MgO and clean MgO, a result of the lack of interaction between Fe and the MgO substrate. The charge density of the surface Fe atoms shows surface-like features typical of metal surfaces, while that of the interface Fe($S-1$) atom shows some influence from the substrate. The layer-projected charge and spin populations of 2Fe/MgO(001) are listed in Table I. The surface Fe atom has a total MT charge of 6.40 electrons or about ~ 0.1 electrons more than of Fe in 1Fe/MgO. The interface Fe($S-1$) atom has a total MT charge of 6.43 electrons, a value very close to that of the surface Fe. Again, the charge population of the MgO substrate atoms is almost unchanged from that of clean MgO or 1Fe/MgO.

The spin density contour plot in the (100) plane of the 2Fe/MgO(001) slab is shown in Fig. 4(b). Large positive spin densities are seen at the two Fe atoms, with a strongly anisotropic shape. Positive spin density appears also at the interface O atom, similar to the 1Fe/MgO(001) results. Negative spin density is seen in the interstitial regions between the Fe atoms. The spin magnetic moment of the surface Fe atoms in 2Fe/MgO is $2.96\mu_B$, which is close in value[12] to that of the free bcc Fe(001) surface atom ($2.98\mu_B$).[11] Very interestingly, the interface Fe has a magnetic moment equal to $2.85\mu_B$, which is smaller than that of the surface Fe by only $\sim 0.1\mu_B$ and is considerably larger than that of the subsurface Fe atom ($2.35\mu_B$) in bcc Fe(001). Compared with the calculated magnetic moment of the bulklike bcc Fe, $2.25\mu_B$,[11] both the surface and interface Fe atoms have strongly enhanced moments (by 32% and 27%, respectively).

The spin-polarized density of states (DOS) of both the surface and interface Fe atoms in 2Fe/MgO(001), plotted in Fig. 5, show similar shapes and energy ranges. For majority spin, the Fe 3d states appear in the energy range -4.0 to -0.5 eV below E_F and the bandwidth is ~ 3.5 eV. There are two high peaks in the DOS at -3.2 eV

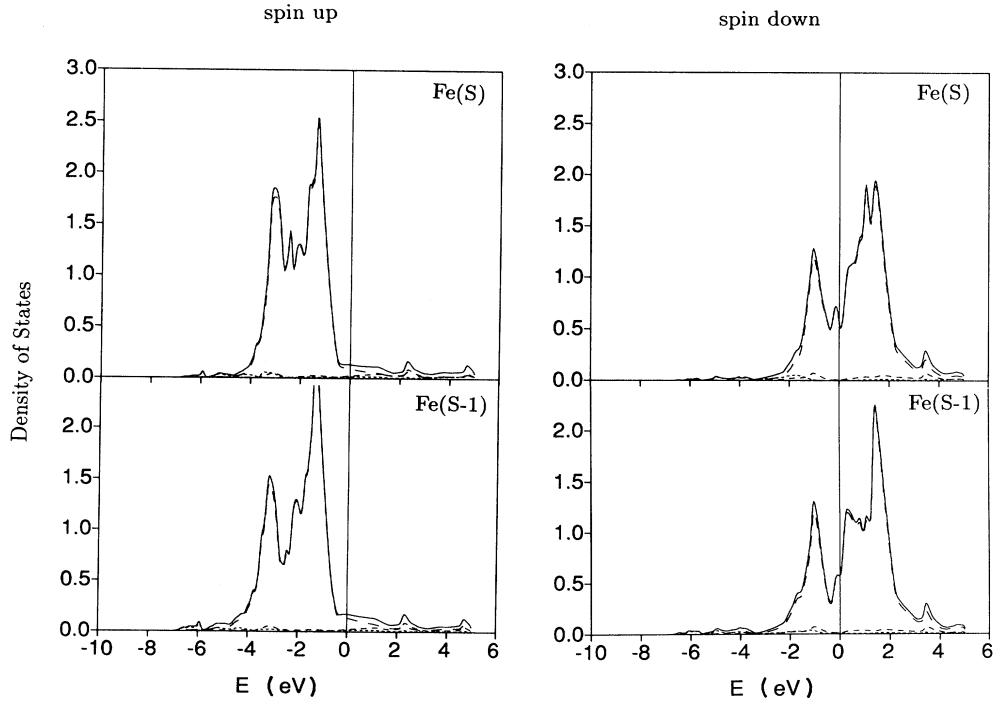

FIG. 5. The layer-projected partial density of states of the conduction electrons for Fe(S) and Fe($S-1$) in 2Fe/MgO(001).

TABLE II. Magnetic moment and the Fermi-contact term of the hyperfine magnetic field at Fe nuclei.

	Total	Valence (kG)	Core	Moment (μ_B)
Free-standing Fe(001) monolayer	−50.8	+393.0	−443.8	3.10
Fe in 1Fe/MgO(001)	−41.9	+396.0	−437.9	3.07
Fe(S) in 2Fe/MgO	−284.2	+135.9	−420.1	2.96
Fe($S-1$) in 2Fe/MgO	−367.9	+36.0	−403.1	2.85
Fe in 1Fe/Au(001) (Ref. 13)	−213	+200	−413	2.97
Surface Fe in bcc Fe(001) (Ref. 11)	−252	+143	−398	2.98
Bulklike bcc Fe (Ref. 11)	−366	−75	−291	2.25

and −1.5 eV for both surface (S) and interface ($S-1$) Fe atoms. Compared with Fe(S), Fe($S-1$) has a slightly larger bandwidth and a higher DOS peak at −1.5 eV. The exchange splitting between the majority and minority spin states is ~2.5 eV. For minority spin, the Fe 3d states appear in the energy range from −1.8 eV below E_F to +2.5 eV above E_F. For both Fe(S) and Fe($S-1$), there are two high DOS peaks at −1.2 eV and +2.0 eV.

D. Hyperfine magnetic field

Finally, the Fermi-contact terms of the magnetic hyperfine field at the Fe nuclei were calculated from the spin-polarized results. They are listed in Table II for 1Fe/MgO(001), 2Fe/MgO(001), and a free-standing Fe monolayer. Also listed in Table II are the results of Ohnishi *et al.*[11] for Fe atoms in a seven-layer bcc Fe(001) slab. Large negative core electron contributions to the hyperfine field are seen in all the systems listed. As expected, the valence-electron (VE) contribution is much more sensitive to the atomic environment than is the core contribution. The total hyperfine field is therefore not proportional to the magnetization–as is seen dramatically in the calculated results.

In 1Fe/MgO(001), the VE contribution gives a large positive hyperfine field (+396 kG), resulting in a small negative net value of the total hyperfine field of only ~−42 kG. This result is remarkably close to that of a free-standing Fe monolayer, but is in sharp contrast with Fe overlayers on Ag(001) or Au(001) substrates[13] in which the total hyperfine field is ~−150 and ~−210 kG for Fe/Ag and Fe/Au, respectively.

In 2Fe/MgO(001), the surface (S) and the ($S-1$) Fe atoms have rather different hyperfine fields. For Fe(S), the total hyperfine magnetic field is −284 kG, a combination of the VE (+136 kG) and core (−420 kG) contributions. This result is somewhat similar to that seen for the bcc Fe(001) surface. The Fe($S-1$) atom has a large value of the total hyperfine field, −368 kG, the result of a much smaller VE contribution (+36 kG).

IV. CONCLUSION

We have investigated the electronic and magnetic structures of both 1Fe/MgO(001) and 2Fe/MgO(001) systems and have found the following.

(i) The MgO(001) forms an extremely noninteractive substrate for Fe thin films; the scale of charge difference induced by the Fe/MgO interface is limited to less than 0.02 e/atom. Thus, Fe/MgO(001) might be an ideal two-dimensional electronic/magnetic system. It is also anticipated that other similar systems, i.e., transition metals interfaced with stable ionic insulating substrates, may yield interesting features of an ideal two-dimensional system. Because of the lack of electronic interaction between Fe and MgO (and possibly in other similar systems as well), we may well have a unique system for studying those properties which are sensitive to the detailed electronic structure. A prime example might be overlayer magnetic anisotropy. We have recently demonstrated[14] that the magnetic moment of monolayer Fe on Ag, Au, and Pd(001) substrates lies perpendicular to the plane of the film, in contrast to the in-plane magnetization found for a free-standing Fe monolayer. Thus, the magnetic anisotropy of a monolayer-range Fe as an overlayer on an MgO(001) should be an interesting test to study experimentally since an in-plane alignment of the magnetization would add considerable evidence for the nearly ideal 2D nature of this overlayer.

(ii) A monolayer Fe adsorbed on an MgO(001) substrate shows a giant magnetic moment (~3.07μ_B), which is remarkably close to that of a free-standing Fe(001) monolayer (~3.10μ_B). This moment is even larger than the previously calculated monolayer Fe moments in Fe/Ag, Fe/Au, and Fe/Cu, etc.

(iii) In 2Fe/MgO(001), the surface Fe atom has a magnetic moment of 2.96μ_B, which is close to that of the bcc Fe(001) surface (2.98μ_B). Surprisingly, even the interface Fe($S-1$) in this system also shows a large magnetic moment (2.85μ_B), which is strongly enhanced over the ($S-1$) moment in bcc Fe(001) (i.e., 2.35μ_b). It also shows a DOS that is extremely close to that of the surface Fe atom. Both findings again indicate the extremely weak interface effect on Fe from the MgO(001) substrate.

ACKNOWLEDGMENTS

This work was supported by the U.S. Department of Energy (Grant No. 88-ER45372) and a computing grant from BES at the Lawrence Livermore National Laboratory Supercomputing Center.

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[12]The 2D lattice constant of MgO(001) is $\sim 3\%$ larger than that of bcc Fe(001). Generally, such expanded lattice constant results in slight enhancement of the local magnetic moment of $3d$ ferromagnetic metals ($\sim 0.02\mu_B$ enhancement at 3% lattice expansion for Fe systems). However, we used a smaller radius, 2.20 a.u., for the Fe atoms in both 1Fe/MgO and 2Fe/MgO (to allow relaxation of the Fe-MgO interlayer spacing), compared with that used in the bcc Fe(001) surface calculation, 2.34 a.u. The change in the magnetic moment of 2Fe/MgO by taking the smaller MT radius is $\sim 0.01\mu_B$. Thus, despite these slightly different factors, the surface Fe of 2Fe/MgO shows no significant difference in magnetic moment compared with that of a free bcc Fe(001) surface atom.
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