PHYSICAL REVIEW B VOLUME 48, NUMBER 2 1 JULY 1993-II

Spin polarization at the Fe/V interface

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(Received 4 February 1993)

The local magnetic moments and magnetic order are investigated at the Fe/V interface of thin Fe_3/V_n films and thin V films adsorbed on Fe substrate. Different crystallographic directions (001), (101), (111), and a two-atom-width and monoatomic-height-per-step stepped surface [corresponding to the vicinal (103) surface] are considered. We calculate the spin-polarized electronic-charge distribution of these systems as a function of the exchange integral J_V of vanadium in the range $0 \leq J_V \leq 0.8$ eV using a self-consistent tight-binding real-space model within the unrestricted Hartree-Fock approximation to the Hubbard Hamiltonian. For (001), (011), and (111) crystallographic faces, the spin polarization of the V atoms at the Fe/V interface is nonzero for any J_V value, with antiferromagnetic coupling between the Fe and V interface atoms. Due to the hybridization between V and Fe orbitals, the spin polarization at the interface tends to increase in V with respect to the corresponding pure-V system, whereas the opposite happens in Fe, resulting in a magnetic moment induced at the interface V atoms by the Fe substrate. This effect is less pronounced in the (101) orientation. Both results can be qualitatively explained by considering two facts: (a) the stronger electron-electron interaction of Fe with respect to V; (b) Fe atoms at the interface have fewer V atoms at nearest-neighbor positions for the (101) orientation than for the (001) orientation. In the case of V adsorbed on the (103) vicinal surface of Fe, the internal and external V atoms at the surface layer of each step are coupled antiferromagnetically. For this particular case, there is a strong competition between the tendencies of V to couple antiferromagnetically with the ferromagnetic Fe substrate and with its V nearest neighbors.

I. INTRODUCTION

Recent experimental and theoretical efforts have addressed the question of a possible onset of ferro- or antiferromagnetism in nanostructures, free-standing clusters, thin-film structures of metals that are paramagnetic in their bulk form. V, Pd, and Rh have been singled out as potential candidates. Considerable studies have been devoted to find the first two-dimensional magnetic metal whose bulk is paramagnetic. Since the experiments of Akoh and Tasaki[1] show the existence of large localized moments in vanadium particles, considerable attention has been devoted to the possible onset of magnetism in free-standing clusters from tight-binding calculations[2,3] or through Stern-Gerlach measurements.[4] Through electron-capture spectroscopy (ECS), Rau, Liu, and Schmalzbauer[5] have detected ferromagnetism at the surface of semi-infinite V(001). Many experiments have explored the magnetic properties of V grown on Ag. Results from ECS (Ref. 6) and surface-impedance measurements of V on Ag(001),[7] inverse photoemission studies of V on Ag(111),[8] superconducting quantum device (SQUID) magnetometer experiments of ultrathin V layers sandwiched in Ag(111) layers,[9] have been interpreted as due to some magnetic moment in the V layer. However, spin-polarized photoemission studies[10] and surface-magneto-optic Kerr-effect[11] (SMOKE) fail to detect unambiguous manifestations of magnetism in ultrathin epitaxial films of V on Ag(001) substrates. Recent photoelectron spectroscopy studies show the appearance of satellite structure in the 3*s* core-level spectra of freshly evaporated V films on graphite,[12] and are interpreted as due to surface magnetic moments. Through full-potential linearized-augmented-plane-wave (FLAPW) calculation, Ohnishi, Fu, and Freeman[13] have shown that a free-standing V(001) monolayer with the bulk-lattice parameter display a ferromagnetic state. With the same method, Fu, Freeman, and Oguchi[14] have obtained ferromagnetism from V epitaxially grown on Ag(001). However, a few years later, Blügel *et al.*[15] with the same FLAPW method were able to display in-plane antiferromagnetism in the V monolayer adsorbed on Ag(001).

Less controversial appears the case where vanadium is in contact with a ferromagnet, as in Fe/V multilayered systems. Multilayered films with artificial superstructures were synthetized by alternate deposition of Fe and V in ultrahigh vacuum.[16] From Mössbauer spectroscopic measurements and polarized neutron-diffraction studies, the reduction of the magnetization at the Fe interface layer is suggested to be about 30%. Analysis of the distribution of the hyperfine field of Fe/V superlattice through a nuclear magnetic resonance (NMR) experiment[17] is compatible with an antiferromagnetic (AF) coupling between Fe and V at the interface, as obtained by Hamada, Terakura, and Yanase.[18] This self-consistent band-structure calculation using the LAPW method was performed for Fe/V layered structure in order to study the distribution of magnetic moments near (001) and (101) interfaces. They found that the magnetic moment per atom of Fe at the interface is appreciably reduced from its bulk value, and that a small negative moment is induced on V at the interface. Conversion electron Mössbauer spectra of composition modulated Fe/V films by Jaggi *et al.*[19] do agree with the results of Hamada, Terakura, and Yanase[18] concerning the decrease of the Fe magnetic moment at the Fe/V interface and the AF coupling between Fe and V at the interface. Recently, Vega *et al.*[20] have discussed, within a tight-binding approximation, the polarization map of Fe_3V_n ($n=1-5$) superlattices for the (001) crystallographic face. A strong antiparallel coupling was found at the Fe/V interface, together with a decrease of the Fe magnetic moment. Contrary to the result of Hamada, Terakura, and Yanase,[18] the polarization of the V layers are AF like, whereas in Hamada's results all the V atoms are polarized in the same direction. This AF configuration is, however, in agreement with the results obtained in bulk vanadium by Moruzzi and Marcus.[21] Investigations of Fe/V films, Fe/V superlattices, and Fe(V) at the surface of a semi-infinite V(Fe) crystal always display antiparallel alignment between Fe and V. Also, it is shown that the interface polarization depends strongly on the crystallographic face considered.

It is the aim of this work to perform a systematic study of the magnetic behavior of these systems composed by V and Fe, in particular, we present calculations of the local magnetic moments and magnetic order at the interface of thin Fe_3/V_n films, and thin V films adsorbed on the Fe substrate. The orientation effect and the local environment effects are discussed by considering different crystallographic directions, (001), (101), (111), and a stepped surface with two-atoms length per step and monoatomic height, corresponding to the vicinal (103) surface. For this purpose, we use a tight-binding self-consistent real-space description within the unrestricted Hartree-Fock approximation to the Hubbard Hamiltonian. This method gives a good representation of the itinerant *d* orbitals of the transition-metal system. This is a reasonable description for transition-metal elements of the middle of the first row like V and Fe (Ref. 22) because the effect of the *sp* electrons in the magnetic moment is less than 10%.[23] This approach has been successfully applied to clusters of Fe, Co, and Ni,[24] and in the case of V slabs and V as an overlayer on Ag(001).[25]

The rest of the paper is organized as follows: In Sec. II, we briefly present our theoretical model pointing out the limit of validity of such parametrized calculation. Section III is devoted to a study of the local magnetic moments and magnetic order at the interface of Fe_3V_n films. Section IV reports the same calculations for V overlayers on semi-infinite Fe. Section V is devoted to the study of a V monolayer on the stepped (103) Fe substrate. Finally, Sec. VI summarizes our conclusions and outlook.

The variety of the magnetic configurations suggests that in experimental work one should look for complex magnetic structures. The main results of this work are the following: (1) The Fe/V coupling at the interface is antiferromagnetic-like. (2) There is an induced spin polarization in V by the Fe substrate, which result in an increase of the magnetic moment at the interface of V, whereas the opposite happens to the Fe interface (Fe with too many V neighbors is nonmagnetic). (3) This effect is less pronounced in the (101) orientation. (4) These results are in agreement with the experimental observations.[16,17,19]

II. THEORETICAL MODEL

The magnetic structure of Fe/V films and V adsorbed on the Fe substrate is calculated by using a self-consistent real-space tight-binding method in the unrestricted Hartree-Fock approximation of the Hubbard Hamiltonian. This Hamiltonian can be written as

$$H=\sum_{i\alpha\sigma}\varepsilon_{i\sigma}\hat{n}_{i\alpha\sigma}+\sum_{\substack{\alpha\beta\sigma\\ i\neq j}}t_{ij}^{\alpha\beta}\hat{c}^{\dagger}_{i\alpha\sigma}\hat{c}_{j\beta\sigma}\ , \tag{1}$$

where $\hat{c}^{\dagger}_{i\alpha\sigma}$, $\hat{c}_{i\alpha\sigma}$, and $\hat{n}_{i\alpha\sigma}$ refer to the creation, annihilation, and number operators of an electron with spin σ at the orbital α of atomic site i ($\alpha\equiv d_{xy},d_{yz},d_{zx},d_{x^2-y^2},d_{3z^2-r^2}$). In the present *d*-band model Hamiltonian,[24] we consider spin-independent hopping integrals, $t_{ij}^{\alpha\beta}$, up to next-nearest neighbors. These elements, $t_{ij}^{\alpha\beta}$, are obtained from the Slater-Koster two-center integrals $dd(\sigma,\pi,\delta)$, which we assume to vary as the inverse of the fifth power of the interatomic distance R_{ij} between ith and jth neighbor atoms:

$$dd(\sigma,\pi,\delta)_{ij}=(6,-4,1)dd\delta_b(R_b/R_{ij})^5\ , \tag{2}$$

where R_b is the corresponding distance in the bulk. They are chosen in order to recover the *d*-band width of Varma and Wilson.[26] We assume that few V overlayers on Fe adopt the substrate's interatomic distance. The lattice parameter of pure V ($a_0^{V}=5.71$ a.u.) is about 5% higher than that of pure Fe ($a_0^{Fe}=5.41$ a.u.). Therefore, we scale the V-V hopping integrals to the Fe lattice parameter accordingly with Eq. (2). Through low-energy electron diffraction (LEED), Jensen *et al.*[27] have observed a 7% contraction of the topmost interlayer spacing with respect to the clean V(001) surface. This contraction is also obtained with the full-potential linear muffin-tin orbital (FP-LMTO) by Methfessel, Hennig, and Scheffler[28] for low-index surfaces of the 4*d* transition metals. For this reason we will take for V, as a first approximation, the hopping integrals corresponding to the Fe bulk lattice parameter. A decrease of the V-V distance means an increase of the hopping integrals,[29] leading to a broadener band. Of course, a more complex approach must be performed, but a more detailed study of the relaxation term is a problem in itself.[28] At the Fe/V interface the two-center hopping $dd(\sigma\pi\delta)_{FeV}$ is approximated by

$$dd(\sigma\pi\delta)_{FeV}=\sqrt{dd(\sigma\pi\delta)_{FeFe}dd(\sigma\pi\delta)_{VV}}\ . \tag{3}$$

The spin-dependent diagonal terms, in the case of Fe_3/V_n films, are given by

$$\varepsilon_{i\sigma}=\varepsilon_i^0+U_i\Delta N_i-\sigma\frac{J_i}{2}\mu_i \ , \tag{4}$$

where i refers to the atomic sites in the system, and σ is the spin. ε_i^0 is the d energy level in the paramagnetic solution of the bulk corresponding to the element (V or Fe) at site i. $U_i\Delta N_i$ takes into account the average shifts in the energy levels, due to intra-atomic direct Coulomb interactions. Here, U_i stands for the effective direct intra-atomic Coulomb integral, and is taken from atomic Hartree-Fock-Slater calculations[30] ($U_V=1.49$ eV, $U_{Fe}=2.33$ eV). $\Delta N_i=\sum_{\alpha\sigma}(N_{i\alpha\sigma}-N_{i\alpha\sigma}^0)$, where $N_i=\sum_{\alpha\sigma}N_{i\alpha\sigma}$ is the average electronic occupation at site i, and $N_i^0=\sum_{\alpha\sigma}N_{i\alpha\sigma}^0$ is the corresponding average electronic occupation in the paramagnetic solution of the bulk of the element at site i. We have chosen $N_i^0=4$ for V, and 7 for Fe, in agreement with the results of Papaconstantopoulos.[31] Finally, the third term in Eq. (4) stands for the shifts due to intra-atomic exchange interactions. The exchange integral J_i for Fe, J_{Fe}, is chosen so as to recover the Fe bulk magnetization ($2.21\mu_B$). In the case of V, there is no possibility to fit this magnitude in the same way as for Fe since V bulk is paramagnetic. On the other hand, there is some uncertainty about the exact value of J_V.[25] Through the linear-muffin-tin-orbital method, Christensen *et al.*[32] have obtained a value of J for all the transition-metal elements (from this calculation it can be deduced the ratio $J_{Fe}/J_V\approx1.46$). However, Stollhoff, Oles, and Heine[33] have shown, using a Hubbard-type Hamiltonian, that the value of J computed in the local-density approximation (LDA) is usually overestimated by 10–20 % because the LDA largely neglects spin correlation. This also led us to consider J_V as a parameter of the calculation.

The number of electrons, N_i, and the local magnetic moments, μ_i, at site i, given by

$$N_i=N_{i\uparrow}+N_{i\downarrow} \tag{5}$$

and

$$\mu_i=N_{i\uparrow}-N_{i\downarrow} \tag{6}$$

are determined self-consistently by requiring

$$N_{i\sigma}=\langle\hat{n}_{i\sigma}\rangle=\int_{-\infty}^{\varepsilon_F}\sum_{\alpha}\rho_{i\alpha\sigma}(\varepsilon)d\varepsilon \ . \tag{7}$$

The energy of the highest occupied state (Fermi energy) ε_F, is determined from the global charge neutrality condition, i.e., the number of electrons per atom in the Fe_3/V_n film must be equal to $(21+4n)/(3+n)$, where n is the number of V layers. Notice that charge transfer between atoms having different local environments may occur. The spin-polarized local density of states (SPLDOS), $\rho_{i\alpha\sigma}(\varepsilon)$, is calculated by means of the recursion method,[34] where the number of levels of the continued fraction is chosen large enough so that the results become independent of it. Twelve satisfies this requirement.

In the case of V layers adsorbed on semi-infinite Fe, the Fermi energy is fixed to the substrate's value, and we impose local charge neutrality ($\Delta N_i=0$) by considering shifts Ω_i in the diagonal terms $\varepsilon_{i\sigma}$. Therefore, in Eq. (4), $U_i\Delta N_i$ is replaced by Ω_i. This approximation has been successfully applied to surface calculations by Victora and Falicov.[35,36] The self-consistent procedure is stopped when the difference between $N_{i\sigma}$(output)$-N_{i\sigma}$(input) is less than 10^{-4}.

III. MAGNETISM IN Fe_3/V_N FILMS

Recently, preliminary results for Fe_3V_n films have been reported.[20] In this previous paper, the V exchange integral, J_V, was taken in accordance with LMTO calculations.[32] A systematical study versus J_V is presented in these more elaborated calculations. Figures 1 and 2 report the results obtained for Fe_3/V_n films for the (001) crystallographic direction. Let us comment on the results.

(i) The magnetic moment at the surface of Fe is greatly increased as compared to bulk iron. This is an usual

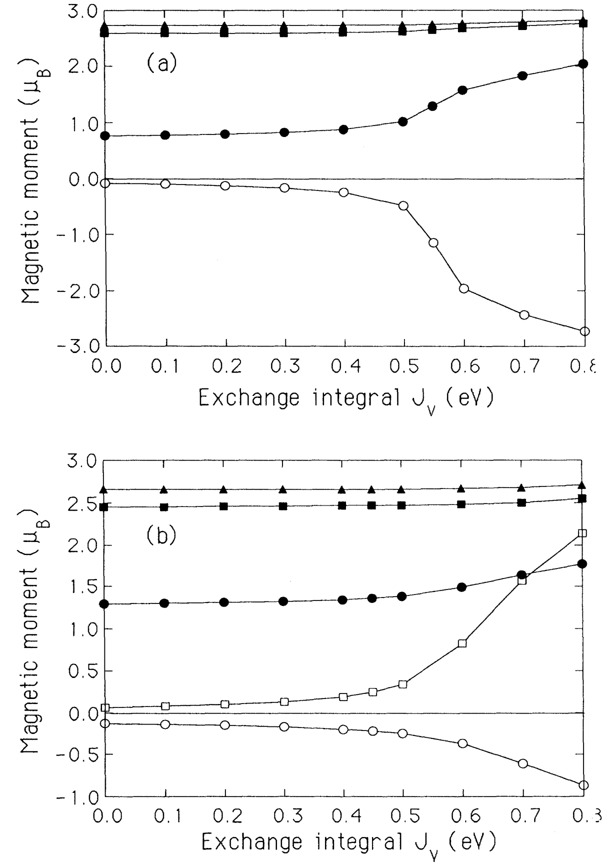

FIG. 1. Magnetic moment μ (in units of μ_B) per atom in terms of the exchange integral J_V, of vanadium for (a) one V monolayer on a three-layer Fe(001) slab: V layer (○), Fe interface (●), Fe central layer (■), Fe surface (▲); (b) two V layers on a three-layer Fe(001) slab: V surface (□), V interface (○), Fe interface (●), Fe central layer (■), Fe surface (▲).

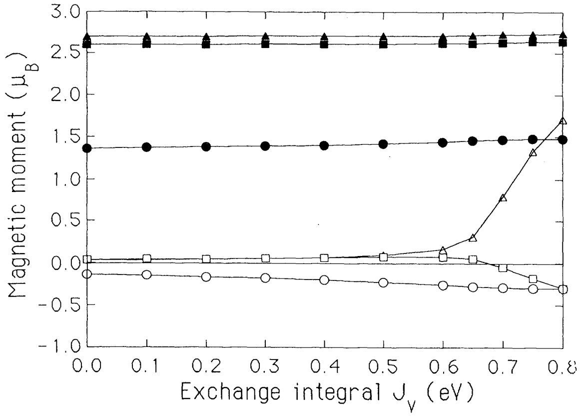

FIG. 2. Magnetic moment μ (in units of μ_B) per atom in terms of the exchange integral J_V of vanadium for a three-layer V slab in contact with a three-layer Fe(001) slab: V surface (△), V central layer (□), V interface (○), Fe interface (●), Fe central layer (■), Fe surface (▲).

phenomenon,[37,38] due to the reduction of the local coordination number at the surface, which led to a narrower *d* band and to the enhancement of the magnetism in Fe.

(ii) At the Fe/V interface, the Fe magnetic moment is drastically reduced as compared to bulk values, whereas an induced magnetic moment on V atoms is obtained. Furthermore, antiferromagnetic-like coupling between Fe and V at the interface is obtained, as in previous calculations.[18,20] The spin polarization of V at the interface for small values of J_V (even for $J_V = 0$ eV, as observed in Fig. 1) is induced by the Fe substrate because there exist no magnetic moments in one free-standing V(001) monolayer for small values of J_V, i.e., for $J_V < J_V^{AF}$, where $J_V^{AF} = 0.25$ eV is the critical value for the onset of magnetism in the free-standing V monolayer.[25] For J_V lower than 0.25 eV, the induced magnetic moment results less than $0.3\mu_B$ (see Fig. 1). For $J_V > 0.25$ eV, there exists a strong increase of the magnetic moments in both V and Fe at the interface. This increase is, however, much faster in V than in Fe because J_{Fe} is fixed whereas J_V increases. The increase of the magnetic moment of V has an effect on the increase of the magnetic moment of the Fe atoms at the interface.

Figures 1(a) and 3 report the results obtained for Fe_3/V_1 slabs for the (001), (101), and (111) crystallographic directions. The following comments can be made.

(i) Whereas for semi-infinite Fe(001), the surface magnetic moment is higher than for semi-infinite Fe(101) [which is a consequence of the larger coordination number of a given Fe atom in the (101) surface plane than in the (001) orientation], when V is adsorbed on these Fe layers to form the Fe_3/V_n films, the Fe atoms at the interface have a smaller magnetic moment for the (001) orientation [Fig. 1(a)] than for the (101) orientation [Fig. 3(a)] if $J_V \leq 0.6$ eV. Analogous trends at the Fe/Cr interface have been reported by Victora and Falicov.[35] A qualitative explanation for this behavior is delayed until Sec. IV, where similar trends obtained for semi-infinite systems V_n/Fe(001) and V_n/Fe(101) will be discussed.

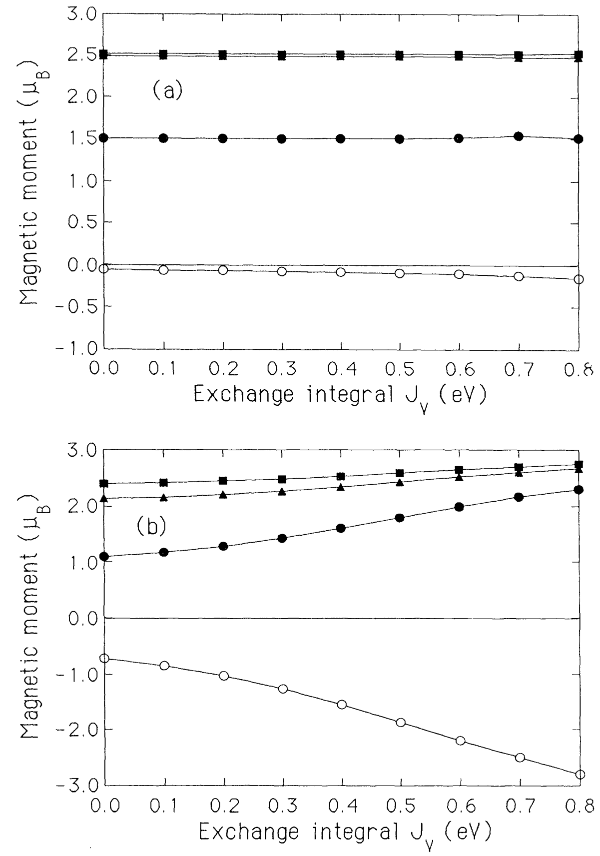

FIG. 3. Magnetic moment μ (in units of μ_B) per atom in terms of the exchange integral J_V of vanadium for (a) one V monolayer in contact with a three-layer Fe(101) slab: V layer (○), Fe interface (●), Fe central layer (■), Fe surface (▲); (b) a V monolayer in contact with a three-layer Fe(111) slab: V layer (○), Fe interface (●), Fe central layer (■), Fe surface (▲).

(ii) The (101) orientation is less favorable for the onset of magnetism since the effective coordination number at the (101) surface is larger than for (001) and (111). In addition, for the (101) orientation there is a strong competition between the tendency of V to couple antiferromagnetically with the Fe substrate and the tendency of each V atom to the antiferromagnetic coupling with its V nearest neighbors.[21,25] This leads to frustration of the magnetism of V and, therefore, to a very small induced spin polarization. However, the antiferromagnetic coupling with the substrate dominates [see Fig. 3(a)].

(iii) The magnetic coupling for the (111) orientation is similar to that obtained for the (001) and (101) crystallographic faces, i.e., ferromagnetic in plane with antiferromagnetic coupling between the V monolayer and the Fe_3 slab [see Fig. 3(b)]. This is the configuration compatible with both the antiferromagnetic tendency in bulk V (Ref. 21) and the tendency of V to the antiferromagnetic coupling with Fe. Furthermore, this orientation is more favorable for the onset of magnetism, as can be observed in Fig. 3(b).

IV. MAGNETIC PROPERTIES OF VERY THIN V FILMS ADSORBED ON LOW-INDEX SURFACES OF Fe

In order to analyze the influence of the thickness of the Fe slab on the spin polarization of the V overlayers, we have calculated the magnetic properties of thin V films adsorbed on Fe substrates at (001), (101), and (111) crystallographic faces. In this case, the Fermi level of the system under consideration is the same as that of bulk Fe and we impose the local charge neutrality condition[35,36,39] as mentioned in Sec. II. The results obtained for V_1/Fe(001) are reported in Fig. 4(a). The spin polarization of the V overlayer is similar to the one obtained in Fe_3/V_1 films. For $J_V=0$ eV, a magnetic moment as high as $0.16\mu_B$ remains at the V layer. Also, the polarization of Fe atoms at the Fe/V interface is considerably reduced as compared to bulk value. Figure 6(a) reports the results obtained for V_1/Fe(101). In this case, for any J_V value up to 0.8 eV, the magnetic moment of the V atoms remains very small. This can be qualitatively explained by considering two facts: on one hand, the larger local coordination number at the (101) surface (this orientation is less favorable for the onset of magnetism), on the other hand, the V atoms in the (101) plane are at nearest-neighboring positions, and the stable magnetic configuration for pure V(101) slabs was obtained in Ref. 25 when the V atoms were antiferromagnetically coupled. However, in the V_1/Fe(101) system, there is a competition effect with the Fe substrate, which tends to be antiferromagnetically coupled with the V overlayer. This leads to frustration of the magnetism of V as in the case of the V_1/Fe_3(101) films discussed in Sec. III. The antiferromagnetic coupling with the Fe substrate dominates in this system [see Fig. 6(a)].

Another interesting point, as already discussed in the case of Fe_3/V_1 slabs, is the considerable reduction of the magnetic moment of Fe at the interface compared to the pure surface case. This reduction is less pronounced in the (101) orientation than in the (001) one. To explain qualitatively this effect, we follow the arguments given by Victora, Falicov, and Ishida[36] for Co/Fe systems. In these calculations, the enhanced magnetization of Fe was attached to the presence of Co which has a stronger electron-electron interaction than Fe. In our V/Fe system, the magnetization of Fe decreases due to the presence of V in its nearest neighborhood, which has a smaller electron-electron interaction than Fe. A further support of this effect is given by neutron-diffraction experiments showing that the Fe impurity in vanadium does not exhibit any magnetic moment[40] contrary to the case of Pd, where one impurity of Fe in Pd leads to a giant magnetic moment.[41] Also, calculations of Fe in V do not present any magnetic moment on the Fe atoms when more than six V atoms are in its neighborhood.[42] Consequently, these experimental[40] and theoretical works[42,43] confirm that the presence of V tends to kill the magnetic moment of Fe. We obtain, in addition, that the magnetic moment of Fe at the interface with V is differently affected by the presence of V for the different orientations. For the (001) orientation, the Fe atoms at the in-

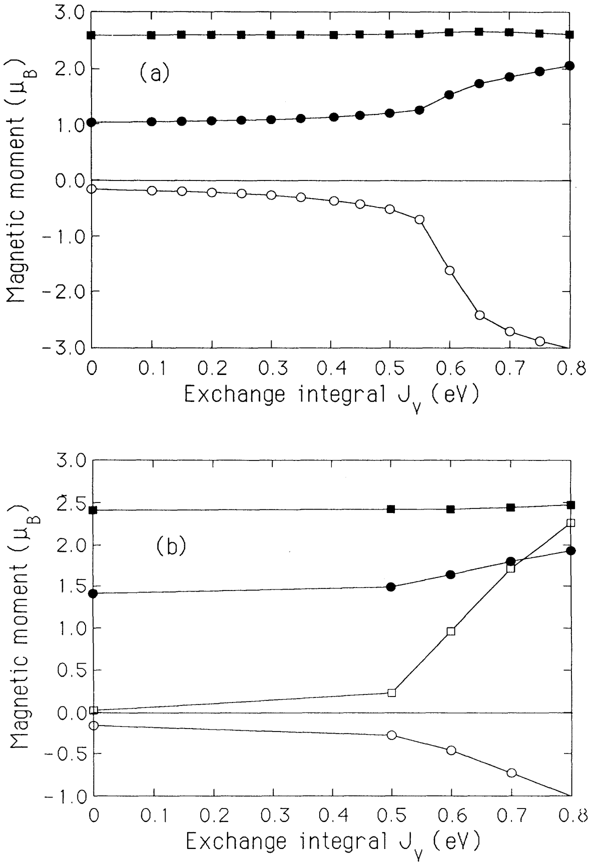

FIG. 4. Magnetic moment μ (in units of μ_B) per atom in terms of the exchange integral J_V of vanadium for (a) a V monolayer on Fe(001) semi-infinite substrate: V layer (○), Fe interface (●), Fe-1 (■); (b) a V bilayer on Fe(001) semi-infinite substrate: V surface (□), V interface (○), Fe interface (●), Fe-1 (■).

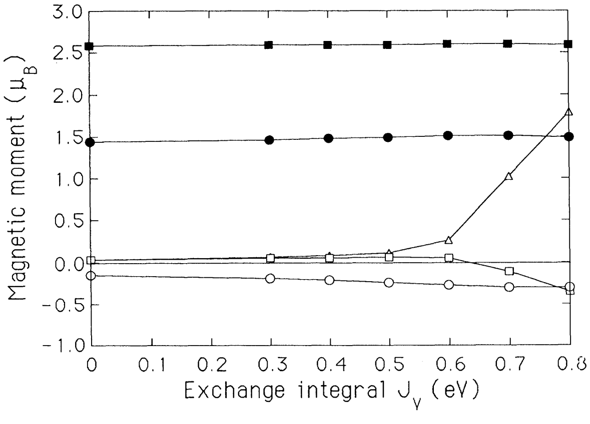

FIG. 5. Magnetic moment μ (in units of μ_B) per atom in terms of the exchange integral J_V of vanadium for a three-layer V slab on Fe(001) semi-infinite substrate: V surface (△), V subsurface (□), V interface (○), Fe interface (●), Fe-1 (■).

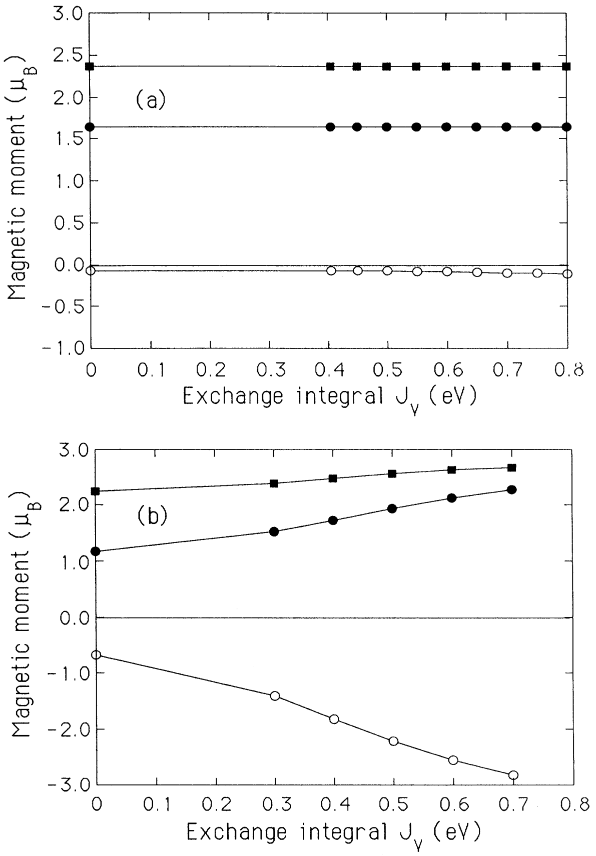

FIG. 6. Magnetic moment μ (in units of μ_B) per atom in terms of the exchange integral J_V of vanadium for (a) a V monolayer on Fe(101) semi-infinite substrate: V surface (○), Fe interface (●), Fe-1 (■); (b) a V monolayer on Fe(111) semi-infinite substrate: V surface (○), Fe interface (●), Fe-1 (■).

terface have four V atoms at nearest-neighbor (NN) positions, whereas in the (101) orientation they have only two V at NN positions. Thus, the magnetic moments at the Fe(001) interface are much smaller than for the Fe(101) orientation.

The results of the V spin polarization obtained in the case of V_n on Fe substrates (Figs. 4–6) are very similar to those of Fe_3/V_n slabs (Figs. 1–3). This seems to indicate that, in these systems, the influence of the Fe substrate on the magnetic properties of the V overlayers is mainly due to the coupling with the first Fe layers.

V. MAGNETIC PROPERTIES OF V MONOLAYER ADSORBED ON Fe(103)

We report in Table I the magnetic moments for the stepped (001) surface of Fe with two-atom length per step and monoatomic height. This atomic configuration corresponds to the vicinal Fe(103) surface. The spin polarization of the Fe atom at the edge of the step (atom 1 in Table I) is the highest of this system. This result is in agreement with torsion oscillation magnetometry experiments performed by Albrecht *et al.*[44] on rough Fe surfaces.

TABLE I. Magnetic moment μ (in units of μ_B) per atom for a stepped Fe surface with two-atom length per step and monoatomic height [vicinal (103) surface]. Results are reported for the internal (2,4) and external (1,3) atoms of the steps in the surface and in the subsurface layer by projection of the system on the (101) plane.

Int.	μ	Ext.	μ
2	2.55	1	2.78
4	2.16	3	2.10

Results for the magnetic moments of the V/Fe vicinal (103) surface are reported in Fig. 7. The spin polarization of the V atom at the edge of the step [atom V1 in Fig. 7(a)] becomes significant for $J_V \approx 0.5$ eV. This value is twice the minimal J_V needed to obtain a magnetic moment for V as an overlayer on Ag(001).[25] This is an unexpected result at first sight because the effective local coordination number of V (taking into account nearest and next-nearest neighbors) is lower in the present

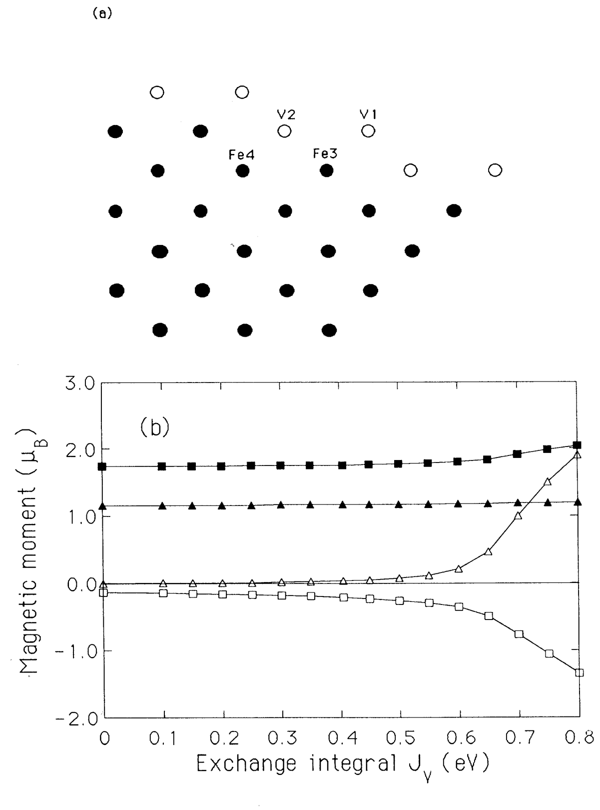

FIG. 7. (a) The stepped surface with two-atoms length per step and monoatomic height [vicinal (103) surface] is sketched by projection in the (010) plane. The Fe atoms are represented by solid circles (●) and the overlayer V atoms are represented by open circles (○). (b) Magnetic moment per atom μ (in units of μ_B) calculated for several values of the exchange integral J_V of vanadium, for the different atoms considered in (a): V1 (△), V2 (□), Fe3 (▲), Fe4 (■).

V/Fe(103) system for V1 [see Fig. 7(a)], than for V at V_1/Ag(001). However, considering that the d orbitals of the V atoms do not hybridize too much with the d orbitals of Ag, the effective coordination number must be recalculated by taking into account only the neighboring atoms (which have a non-negligible amount of hybridization with V). This leads, for V at the edge of V_1/Fe(103) [V1 in Fig. 7(a)], to a much higher effective coordination number than in the case of V adsorbed on Ag(001) and thus to an onset of magnetism for a much higher J_V value than in the case of V on Ag(001).

From Fig. 7(b), two regimes of magnetization as a function of J_V can be inferred.

(i) For $J_V < 0.5$ eV, the V atom at the edge [V1 in Fig. 7(a)] does not show a measurable magnetic moment, whereas the magnetic moment of the V atom at the internal position of the step [V2 in Fig. 7(a)] increases very slowly. This magnetic moment in V2 is mainly due to the spin polarization induced by the Fe substrate. Note that the internal V atom (V2) has more Fe neighbors than the external V atom (V1) and thus a higher spin polarization for small J_V.

(ii) For $J_V > 0.5$ eV, the magnetic moment of the V atom at the edge increase rapidly, so that for $J_V = 0.66$ eV it becomes larger (in absolute value) than the moment of the V internal atom, of type 2. This kind of behavior, where the external atom has a bigger magnetic moment than the internal one, has been found previously in the case of V films.[25] In the present case, the situation is a little bit different because the induced magnetic moment arising from the Fe underlayers is predominant for small J_V. This is no longer the case when J_V is high.

We now wonder why the configuration with parallel magnetic moment alignment for the V atoms does not appear. Observe that a V atom of type 2 is antiferromagnetically coupled with Fe because it has mainly Fe atoms in its neighborhood, whereas a V atom of type 1 has the same number of V and Fe atoms in its neighborhood. The result is an AF coupling between the V atoms of types 1 and 2 [see Fig. 7(a)] in this particular case. The stepped surfaces with n-atom ($n = 2,3,4,\ldots$) length and monoatomic height correspond to the vicinal surfaces $(1,0,2n-1)$. Results in Fig. 7(a) correspond to the stepped surface with $n = 2$. When the number of atoms n increases infinitely, the vicinal surface reaches the low-index (001) surface. In this case, all the V atoms are polarized ferromagnetically, whereas the coupling with Fe is antiferromagnetic-like. When $n = 1$, the vicinal surface reaches the low-index (101) surface, where the same magnetic ordering as for (001) has been found [see Fig. 6(a)], thus indicating that the antiferromagnetic coupling between V and Fe dominates in both systems. This is no more the case when the steps are present as in V_1/Fe(103) [see Fig. 7(b)]. The different geometrical and chemical environment of the internal (V2) and external (V1) V atoms of the step leads to a very different local density of electronic states in these atoms. In particular, the electronic occupation at the Fermi energy is lower for the internal atom (V2), whereas the electronic state's degeneration at the Fermi energy is higher for the external atom (V1). Following the Stoner criterion, the magnetic energy gain when these atoms are polarized is expected to be larger for V1 than for V2. These facts indicate the importance of the geometrical and chemical local environment on the magnetic structure of these systems.

VI. SUMMARY AND OUTLOOK

A self-consistent calculation of the local magnetic moments and magnetic order of Fe_3/V_n films and thin V films adsorbed on Fe substrates with different crystallographic faces has been presented. The ground-state electronic structure has been described within the unrestricted Hartree-Fock approximation of the Hubbard Hamiltonian and has been determined for several values of the exchange integral of V in the range $0 \le J_V \le 0.8$ eV. For (001), (101), and (111) orientations we obtain nonzero spin polarization in the V atoms at the Fe/V interface even for $J_V = 0$ eV, together with an antiferromagnetic coupling between V and Fe at the interface. Due to the hybridization between V and Fe orbitals, the spin polarization increases (decreases) for V (Fe) atoms at the interface. This fact leads to an induced magnetic moment in the V atoms by the Fe substrate which is less pronounced in the (101) orientation. Both results are qualitatively explained by considering two facts: (i) the stronger electron-electron interaction of Fe with respect to V; (ii) Fe atoms at the Fe/V interface have less V atoms at nearest-neighbor positions for the (101) orientation than for the (001) one, so that the decrease of the Fe magnetic moment is less pronounced for the (101) orientation.

These results are in agreement with the experimental observations[16,17,19] for analogous systems and first-principle calculations.[43] In the case of V adsorbed on the (103) stepped surface of Fe, the internal and external V atoms at the surface layer of each step are antiferromagnetically coupled, indicating that such a type of roughness (two-atom length steps) tends to kill the average magnetization at the V monolayer adsorbed on Fe. Therefore, it would be interesting to perform spin-resolved photoemission experiment measurements in order to test this proposal.

ACKNOWLEDGMENTS

This work was supported by DGICYT (Spain), Junta de Castilla y León, and Acciones Integradas Hispano Francesas.

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