Effect of hydrogen on the interlayer exchange coupling in Fe/V superlattices

S. Ostanin, V. M. Uzdin, C. Demangeat
IPCMS-GEMME, 23, rue du Loess, F-67037 Strasbourg Cedex, France

J. M. Wills
Center for Materials Science and Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87544

M. Alouani and H. Dreyssé
IPCMS-GEMME, 23, rue du Loess, F-67037 Strasbourg Cedex, France
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Electronic and magnetic structures of Fe/V superlattices with and without hydrogen in the vanadium spacer are investigated using a relativistic full-potential linear muffin-tin orbital method. We obtained short-range induced spin polarization in V as well as reduced Fe polarization at the Fe/V interface. The value of the magnetic moment induced on the vanadium atoms depends strongly on the distortion caused by the lattice mismatch and hydrogen loading whereas the total moment of the Fe and V interface layers remains almost unchanged. Hydrogenation of the V spacer leads to the decrease of the interface magnetic moment on the V atoms and to a reduction of the density of states (DOS) at the Fermi level. A low DOS could be one of the reasons for the experimental increase of the resistivity of the samples under hydrogen loading and leads to the disappearance of the antiferromagnetic exchange coupling in the Fe/(VH) superlattices for large hydrogen concentration. Doping the V film by a gold monolayer increases the DOS at the Fermi level and could recover the antiferromagnetic coupling.

I. INTRODUCTION

The interest to the magnetic properties of the multilayers with V spacers was stimulated recently by the possibility to change in a relative simple way the electronic and magnetic structures of the V layers. Such changes governed by the lattice mismatch in the superlattices or by the introduction of hydrogen into the V spacer open a new way for the manipulation of the interlayer exchange coupling (IEC) in the multilayers.

Bulk V is a nonmagnetic metal. However, calculation gives the transition to the antiferromagnetic (AF) state[1] when the lattice constant increases by 23%. Lattice constant of V can be changed by contact with material having larger lattice constant like in Mo/V superlattices[2] or by introducing hydrogen which penetrates in the V layers only and leads to an essential increase of the interatomic distance.[3] There are, however no experimental evidences of the V transition into the magnetic state even in the case of lattice expansion up to 10%.

The small V clusters and even the monolayers supported on the surface of nonmagnetic metal have localized magnetic moments. Shintaku *et al.*[4] observed, using super conducting quantum interface device magnetometer the existance of magnetic moments in ultrathin V layers sandwiched in Ag layers. Weber *et al.*[5] performed the calculation for small free standing and supported V clusters in *ab initio* Green's function technique and found magnetic moments greater than 2 μ_B per V atom. In the FeV alloys[6] and in the interface region of the Fe/V multilayers[7,8] magnetic moment on V atoms due to the Fe-V interaction was measured. The augmented spherical wave[9] (ASW) and the tight-binding linear muffin-tin orbital[10] (TB-LMTO) methods reported nonzero-magnetic moments at the interface V atoms but the value of the moment on the second from the interface layer is almost zero. Interface roughness and distortion essentially influence the value of the moment and it can be important for the understanding of the coupling phenomena in the superlattices.

IEC through the vanadium spacer in epitaxial Fe/V superlattices was detected and characterized only recently. Granberg *et al.*[11] investigated Fe/V (001) superlattices with thicknesses of V layer from 1 to 12 monolayers (ML). For all the thicknesses the system shows ferromagnetic (FM) coupling. Similar behavior without signature of an AF IEC was found by Schwickert *et al.*[8] for the sputtered Fe/V superlattices with thin (less then 13 ML) V spacers although superlattices with larger thicknesses of the V spacer show oscillation of the IEC. Poulopoulos *et al.*[12] found for the superlattices with a V interlayer thickness of 13 ML an hysteresis loop with bilinear and biquadratic IEC features. The Fe_3/V_l superlattices were investigated using spin-polarized neutron reflectivity[13] and by longitudinal magneto-optical Kerr effect[14] and for l varying from 12 to 14 ML the AF IEC was found.

Hjörvarsson *et al.*[13,14] have shown that the IEC in the Fe/V superlattices can be switched from AF to FM and vice versa upon introducing hydrogen to the V layers. Loading of the hydrogen leads to the expansion of the vanadium spacer layer. The total thickness of the V layer can be changed reversibly by as much as 10% at moderate H pressures without any memory effects.[3] Within a free electron model it leads to the change of the thickness of the quantum wells for the electron with different spin projection on the direction of magnetization in the magnetic layers and, correspondingly to the short-range oscillations of the IEC.[15] The Fe_3V_l superlat-

tices that were investigated in experiment[13,14] had a thickness l of the V spacer between 11 to 16 ML. Without hydrogen they show AF IEC for l between 12 and 14 ML. Hydrogen loading leads in these superlattices to the sharp transition to FM coupling. In the structures with $l=15$ and 16 ML introduction of H induces an AF ordering for a narrow concentration range. However further increase of the hydrogen concentration destroyed the AF IEC. So, for high-hydrogen concentration AF IEC was suppresed in in all the superlattices. It means that the influence of H on IEC cannot be explained only by the change in the V thickness. Therefore, detailed information on the electronic and the magnetic structure of the V spacer under hydrogenation is needed for the explanation of the experiments.[13,14]

In the present paper, we investigate the electronic and magnetic structures of the Fe/V multilayers with hydrogen in V spacer using the relativistic full-potential linear muffin-tin orbital (FP-LMTO) method.[16] We will focus on two questions. The first is the role of the lattice expansion and of the tetragonal distortion in the V layers on the formation of the magnetic structure in V/Fe superlattices. The bulk lattice mismatch between Fe and V is about 5.1% so that the in-plane biaxial strain of the V layers is compressive. It leads to an increase of the in-plane lattice constant of the Fe layers and consequently to an enhancement of the Fe magnetic moments due to the decrease of the *d*-band width. The V layers, on the contrary, will have smaller lattice constant in plane but perpendicular to the plane the interatomic distance will be larger than in the bulk. Hydrogen induces additional expansion of the lattice and as was shown by Andersson *et al.*[3] for Fe/V multilayers, only in perpendicular-to plane direction. So, in Fe/V superlattices we have very specific structures with large tetragonal distortion and calculations based on the atomic sphere approximation[8–10] may be dubious.

The second question is connected with the modifications of the electronic structure of the V spacer in the superlattice under adsorbed hydrogen. Calculations of the structural and the electronic properties of the bulk VH_x ($x=0,0.5,1.0$) was performed within FP-LMTO method by Andersson and co-workers.[17] When the octahedral O_z sites of bulk VH_x system are occupied by hydrogen the V-H interaction moves the Fermi level into the density of states (DOS) dip.[17] The presence of the Fe layers leads to the hybridization of Fe and V states and to the appearance of induced magnetic moments at the interface V layers. How much this induced polarization will be modified by hydrogen loading and what will be the resulting electronic structure of Fe/VH_x is an open question. These two points have to be solved in order to find an explanation of the behavior of the IEC in Fe/V multilayers with H in V spacer.

The paper is organized as follows. In Sec. II, we describe briefly the first-principles method used and the computational details. Section III includes our results and discussion. Finally, in conclusion, we summarize the ability of our model to interprete the experimental data.

II. THEORETICAL MODEL

The available measurements of the IEC in the Fe/V superlattices with hydrogen in V spacer were performed for the Fe_3V_l structures, where the thickness of the Fe layer was fixed at three monolayers whereas the number l of V monolayers varies from 11 to 16 ML. Previous calculations of the Fe/V multilayers[9,10,18] show that the induced magnetic moments in the V spacer decreases very fast with distance from the interface and that on the 2nd–3rd from the interface layers it became practically equal to zero. Our calculations for superlattices with 7 and 9 ML of vanadium in the FP-LMTO method with different kind of distortion also give neglegible magnetic moment and very similar electronic structure for all V atoms beginning from the third from the interface layer. So, in what follows we will discuss only the Fe_3V_5 superlattices taking into account that for thicker V spacer inner V layers are nonmagnetic and have electronic structure similar to that of the central V layer in Fe_3V_5 system.

The electronic structure is calculated by a relativistic FP-LMTO method[16] within the generalized gradient approximation[19] (GGA) to the exchange-correlation potential in the framework of the density-functional theory. The GGA improves considerably the quantitative agreement of the calculated bulk equilibrium volume with the observed one.[20] The spin-polarized electronic states of the core electrons are calculated by solving iteratively the Dirac equation. For the valence electrons the spin-orbit coupling is added to the scalar-relativistic Hamiltonian. The magnetization axis is chosen along the [100] direction in superlattice's plane. The electron density and potential were expanded in spherical harmonics up to $L_{max}=6$ inside the nonoverlapping muffin-tin spheres centered on each atom. The potential for the interstitial region is obtained by using the fast Fourier transformation and the real space grid is $16\times16\times16\cdot n$ (n is the ML number). Our results are converged in the number of k points of the Brillouin zone as well in the number of tails of basis functions in the interstitial region. The Gaussian smearing function of 7 mRy width is chosen to improve the convergence in the 128 $\vec{k}$-point sample in the irreducible part of the Brillouin zone. To calculate the spin-resolved partial DOS a converged potential together with the tetrahedron method are used.

The sites in the unit cell of the Fe_3/V_5 (100) superlattice are shown in Fig. 1. Three types of model superlattices were selected to describe the tetragonalization of the films under experimental investigation:[13,14] (i) the perfect bcc structure with in-plane lattice parameter which corresponds to the experimental value of bulk Fe ($a_{\parallel}=2.87$ Å), (ii) the bct structure with the in-plane lattice constant of bulk Fe while the ratio of out-of-plane parameter $c=a_{\perp}$ to $a_{\parallel}$ is changed from $c/a_{\parallel}=1$ for Fe layers to $c/a_{\parallel}=1.1$ for V layers, and, finally, (iii) the bct lattice with in-plane lattice parameter of bulk V and $c/a_{\parallel}=1$ and 1.1 for Fe and V layers, respectively. The out-of-plane interface parameter between Fe and V is always a mean value of the two $a_{\perp}$ constants. The value of the tetragonal distortion of the V ML corresponds to the maximal measured c/a ratio for Fe_3/V_l (100) superlattice under hydrogenation.[3] The muffin-tin radii of the V and Fe atoms were kept the same for each supercell but for different supercells (Fig. 1) it was modified in order to keep the same ratio between the interstitial and the total volume of the supercell. Such a model allows us to investigate the effect of tetragonalization on the interface magnetism and the magnetic behavior of the V spacer in Fe/V superlattices. Calculations of the electronic and magnetic structures of bct

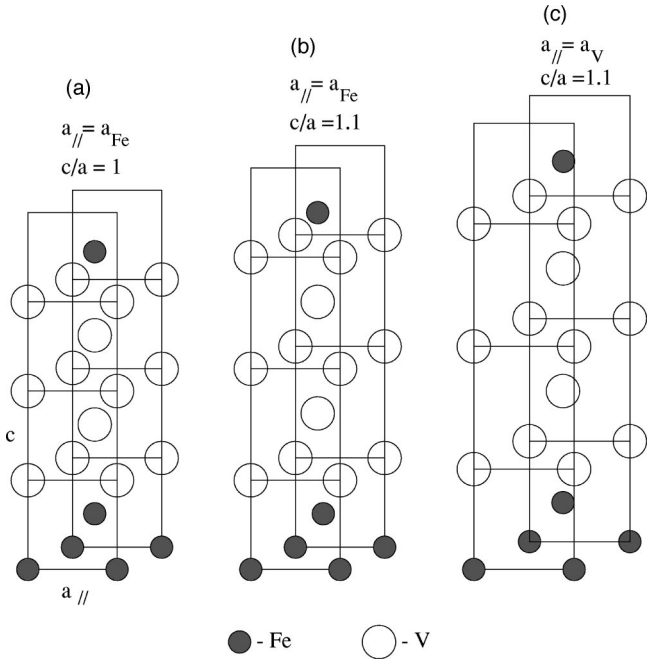

FIG. 1. Unit cell of the tetragonally distorted and nondistorted Fe_3/V_5 (100) superlattices: (a). bcc supercell with the lattice parameter of bulk Fe; (b). bct supercell with the in-plane lattice parameter $a_\parallel$ of bulk Fe and the tetragonal distortion of V spacer $c/a=1.1$; (c). bct supercell with the in-plane lattice parameter of bulk V and the tetragonal distortion of V spacer $c/a=1.1$.

Fe_3/V_5 superlattice with hydrogen are performed for supercell shown in Fig. 2.

The z direction in Fig. 2 is perpendicular to the (100) surface. We restrict our consideration to the specific type of $a_\parallel^{\mathrm{Fe}}$ and $c/a=1.1$ for tetragonally distorted V spacer. This value of the distortion corresponds to the measurements of

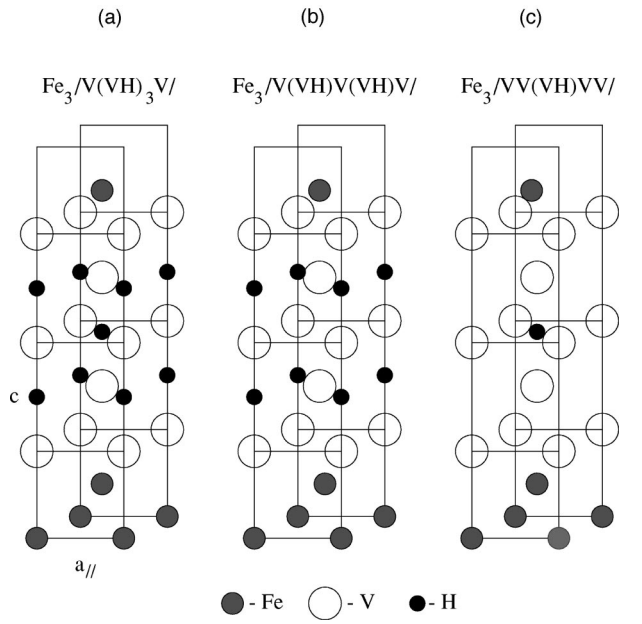

FIG. 2. Unit cell of the tetragonally distorted Fe_3/V_5 (100) superlattices under hydrogenation: $a_\parallel$ is the Fe bulk lattice parameter while $c/a=1.1$ for the V spacer. The interstitial H atoms are shown at the different octahedral O_z sites.

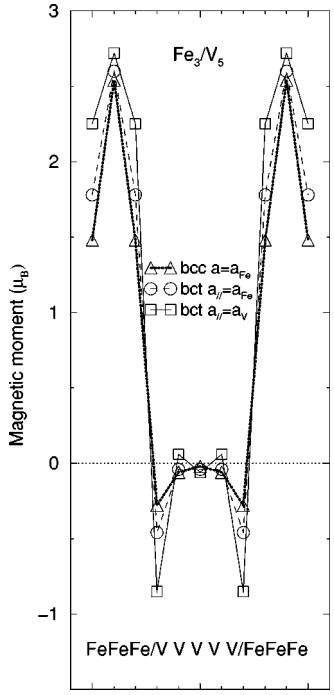

FIG. 3. Calculated layer-resolved spin moments of the Fe and the V atoms for Fe_3/V_5 (100) superlattices. Thick dotted line joining triangles corresponds to the bcc supercell with the $a_\parallel$ of the bulk Fe [Fig. 1(a)]; dashed line (open circles) corresponds to the bct supercell with the $a_\parallel$ of the bulk Fe and $c/a=1.1$ for the V layers [Fig. 1(b)]; thin-solid line joining squares corresponds to the bct supercell with the in-plane lattice parameter of bulk V and $c/a=1.1$ [Fig. 1(c)].

the expansion coefficient in Fe/V (100) single crystal system performed by Andersson and co-workers.[3] This expansion coefficient depends strongly on the average H/V (atomic ratio) concentration c_H. At $c_H\sim 0.5$, the c/a ratio is ~ 1.09. Andersson and co-workers connect this strong tetragonalization effect with the occupancy of the octahedral O_z type sites by the hydrogen atoms.

In order to investigate the magnetic properties of the hydrogenated Fe/V (100) superlattices vs H concentration we modify the O_z sites population as shown in Fig. 2. The c_H starts from 0.2 [Fig. 2(a)] and increases up to $c_H=0.6$ [Fig. 2(c)]. The muffin-tin radii for vanadium and hydrogen were optimized and found to be related by $r_{MT}^H/r_{MT}^V=0.3$.

III. RESULTS AND DISCUSSION

A. Spin moment versus strain in Fe_3V_5 superlattices

A starting point of our investigation of the Fe/V superlattices is an illustration of pure strain effect. We plot in Fig. 3 the layered-resolved spin magnetic moment for the three types of supercells shown in Fig. 1. The bcc Fe_3/V_5 (100) superlattice with the bulk Fe lattice constant, shows a spin magnetic moment of 2.54 μ_B on the central Fe ML. It is essentially larger then the one reported for inner Fe layers in Fe_n/V_l ($n\geqslant 5$) superlattices.[9,10] The bct distortion, which in our case means the increase of the $a_\perp$ lattice constant in the V spacer leads only to an increase of the moment on the central Fe layer. The reason for such an enhancement lies in the chemical arrangement of the system under consideration.

Previous calculations[9,10] have reported small increase of the moments for the second from the ideally sharp interface Fe layer in Fe/V multilayers. The central Fe layer in the Fe_3/V_5 superlattice has next-nearest-V layers at both sides. So, the moments on this Fe layer should be enhanced relatively to the moment of the second from the interface Fe layer in the Fe/V superlattices with larger thickness of Fe slabs. However observation of this enhancement requires very smooth interface without alloying and very special experimental methods, which provide local information about magnetic structure. A similar increase of the magnetic moments for the Fe atoms having Cr among its second neighbors was predicted in Fe/Cr multilayers[9] and for Fe clusters embedded in Cr.[21] However, enhancement of the hyperfine fields at the Fe nuclei relative to the bulk value, which is connected with these increased moments, was found only for specially prepared epitaxial samples[22] with suppressed alloying and was never reported in sputtered samples.[23]

Magnetic moments of the Fe atoms at the interface with V are smaller than in the bulk Fe. The values of the moments for these atoms are more sensitive to distortion than the moments of the central Fe layer. This is connected with the increase of the distance to the nearest V atoms due to distortion and has the same origin as the enhancement of the magnetic moments near the Fe surface.[24] Previous band-structure calculations[9,10,18] displayed similar results with Fe magnetic moments between 1.5 μ_B and 1.8 μ_B at the interface with V. The values of the Fe magnetic moments reported in the experimental papers are essentially less then those obtained by the theoretical predictions. Poulopoulos *et al.*[12] have found that the Fe magnetic moment is reduced to 0.7 μ_B. For the inner Fe layers they found a magnetic moment equal to the moment of bulk Fe. Labergerie *et al.*[14] concluded from the magnetization experiments that for the Fe_3/V_l; ($l=11-16$) superlattices not only the boundary layers exhibit a reduced moment (0.7 μ_B) but also the interior Fe layer.

The discrepancy between the theory and the experiment needs more careful considerations. Poulopoulos *et al.*[12] estimated the value of the Fe magnetic moments using the linear dependence of the saturation magnetization in Fe_n/V_l superlattices (per Fe volume) to the inverse of the number of Fe layers *n*. They completely neglected the polarization of the V layers in accordance with Granberg *et al.*,[11] who wrote that it is only 1–2% of the total magnetization of the Fe slabs. However Granberg and co-workers[11] considered the superlattices with 15 ML in the Fe slabs. For the superlattices with 3–5 Fe monolayers the contribution of the V layer to the total moment will be much more essential. So, effectively Poulopoulos *et al.*[12] estimated not the moment of the interface Fe layer but the difference between Fe and V interface moments due to AF Fe-V coupling.[12] Another important point which was not taken into account in Ref. 12 is the interface alloying. As was shown by calculations within ASW method[8,9] alloying at the interface increases the polarization of V and decreases the moments on the Fe atoms. Obviously this effect will be especially important for superlattices with thin Fe slabs. Therefore, the small value of the magnetization in the experiments of Labergerie *et al.*[14] is most probably the signature of the alloying, which cannot be avoided for 3 ML Fe films.

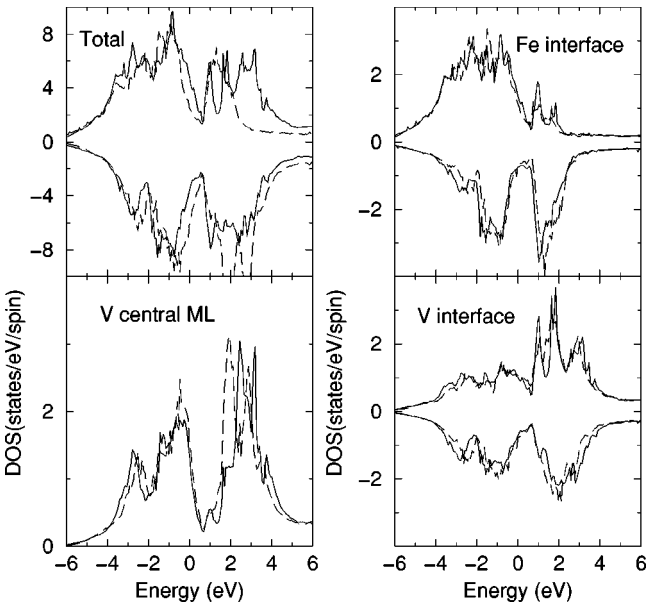

FIG. 4. The spin- and layer-resolved DOS of Fe_3/V_5 (100) superlattices for $a_\parallel$ of the bulk Fe. Solid and long-dashed lines correspond to the bcc [Fig. 1(a)] and bct [Fig. 1(b)] supercells, respectively $E_F=0$.

The V atoms have sizable induced magnetic moments only at the interface layer with Fe (Fig. 3). This moment is antiparallel to the Fe magnetization direction in accordance with experimental data[7] and previous calculations.[9,10,18] The value of the V moment depends strongly on the distortion. An increase of the lattice constant enhances the induced polarization of the V atoms, as well as the Fe magnetic moments. The total moment of the superlattice, which includes the moments of the Fe layers and of the interface V layers, depends very weakly on the distortion, although the individual moment at the interface V atoms indicates a more pronounced change (Fig. 3).

Distortion in epitaxial Fe/V superlattices can be governed by the choice of the number of Fe and V layers. Within the linear elasticity approach, the biaxial strain state is expected to scale linearly with the ratio of the constituents' thicknesses.[3] However, contribution to the saturation magnetization from the interface layer remains almost constant and does not depend on the thicknesses of the Fe and the V films. This point is important to accounts for the interpretation of the linear correlation between saturation magnetization in the Fe/V superlattice and the inverse number of Fe layers in each Fe film.[12]

In Fig. 4, we display the spin-resolved DOS of the perfect bcc and tetragonally distorted bct Fe_3/V_5 (100) superlattices, corresponding to the same $a_\parallel^{Fe}$ lattice constant [see Figs. 1(a) and 1(b)]. The shape of the DOS has many points in common with the DOS for the FeV-disordered alloy.[25] In particular, for the Fe interface layer, the Fermi level resides in the bonding-antibonding valley of the minority spin. The position of this valley is not modified by tetragonal distortion. In the total DOS the Fe component dominates the occupied *d* bands while the V DOS component indicates a pronounced multipeaks *d* structure around 2 eV above the Fermi level. It is this multipeaks structure that changes es-

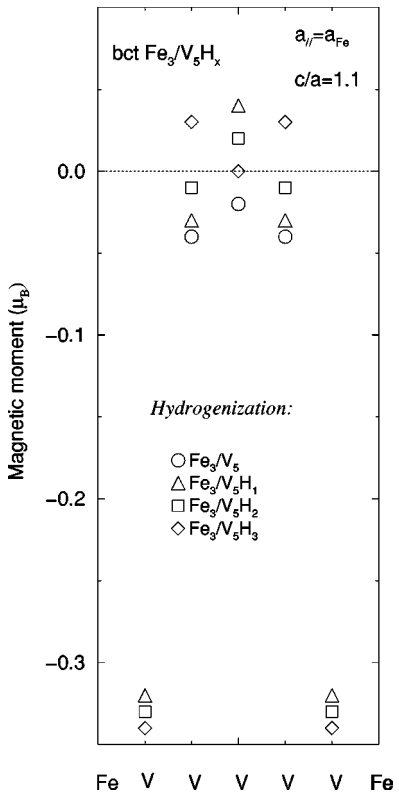

FIG. 5. Calculated layer-resolved spin moments of V atom of bct Fe_3/V_5 (100) superlattices for $a_{\parallel}^{Fe}$ and $c/a=1.1$ under hydrogenation. Open circles correspond to non-hydrogenated supercell, triangles to the $Fe_3/V_2(VH)V_2$ [Fig. 2(c)], squares to the $Fe_3/V(VH)V(VH)V$ [Fig. 2(b)], and diamonds to the $Fe_3/V(VH)_3V$ [Fig. 2(a)], respectively.

sentially under distortion. These states, however are not occupied and do not influence the magnetic properties of the V spacer.

B. Electronic structure of the FeV multilayers under hydrogenation

In this section, we will consider the changes of the electronic and magnetic structures of Fe/V superlattices under hydrogenation. Experimentally it was detected[3] that hydrogen in FeV multilayers penetrates only into the V spacer and moreover a few (two or three) V monolayers at each interface do not dissolve hydrogen to the same extent as the interior layers. Loading of the hydrogen is accompanied by the extention of the V spacer perpendicular to the superlattice's plane direction and by the increase of the resistivity of the superlattice.[3]

We performed the electronic structure calculations of the superlattices Fe_3/V_5H_x $(x=1,2,3)$ which are shown on Fig. 2. Concentration $c_H=\langle H\rangle/\langle V\rangle$ of the hydrogen in the V layers corresponds to 0.2, 0.4, and 0.6. The calculated layer-resolved spin moments of V atoms are displayed on Fig. 5. Moments of the inner V atoms changes slightly under hydrogenation but their values do not exceed 0.05 μ_B. The moment of the interface V atoms decreases from 0.48 μ_B without hydrogenation (Fig. 3) to 0.32 μ_B for $c_H=0.2$ and then slightly increases versus hydrogen concentration until 0.34 μ_B for $c_H=0.6$ (Fig. 5). Similar but more pronounced

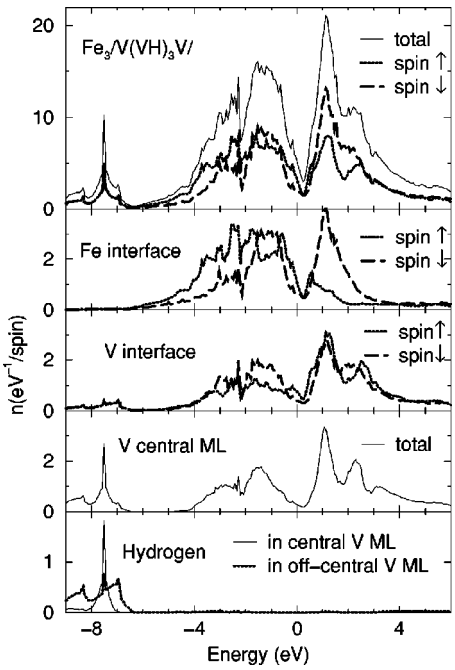

FIG. 6. Total and layer-resolved DOS of bct $Fe_3/V(VH)_3V/(100)$ superlattice with in-plane lattice parameter of bulk Fe and $c/a=1.1$ [Fig. 2(a)].

variation of the magnetic moments takes place at the Fe interface. The Fe moments at first decrease from 1.72 μ_B ($c=0$, Fig. 3) to 1.56 μ_B for $c_H=0.2$ but than again increase: 1.65 μ_B for $c_H=0.4$ and 1.72 μ_B for $c_H=0.6$. So, for high-hydrogen concentration, the interface Fe atoms have almost the same magnetic moment as without hydrogenation. The magnetic moments of the central Fe layer remains practically unchanged.

Andersson *et al.*[17] proposed that it should be possible to produce magnetic V by a combination of hydrogenation and the growth of overlayers or multilayers with Mo, having larger lattice constant. Our calculations show that despite the distortion, the polarization of the interface V layers in Fe/V superlattices decreases after hydrogen loading. Therefore, hydrogenation of the nonmagnetic Mo/V multilayers will probably not give a magnetic moment on V atoms.

Figure 6 displays the spin- and layer-resolved DOS of the hydrogenated superlattice for $c_H=0.6$. The hydrogen $1s$ states are located at around 8 eV below the Fermi level ($E_F=0$). The hybridization of these states with the d bands of V is localized in real space: only the inner V atoms have peaks at energy around -8 eV. A similar peak was found by Andersson *et al.*[17] for the bulk VH_x ($x=0.5$ and 1). The interface V layers with Fe do not contain hydrogen and show very small DOS below -4 eV relative to E_F. The Fe atoms change their state under hydrogenation only indirectly through the hybridization with V neighbors.

An interesting detail that is important for the understanding of the properties of the superlattices under hydrogenation is the pinning of the V DOS at the Fermi level. In order to trace the origin of this low DOS on Fig. 6 we plotted the layer-resolved DOS of the central V layer in the Fe_3V_5 superlattice for different concentrations of hydrogen in the V spacer. The deep valley, which for the superlattice without hydrogen, was located at 0.5-1 eV above the Fermi energy

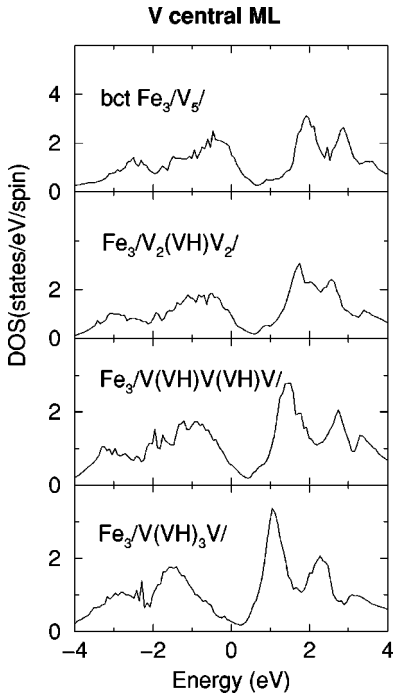

FIG. 7. The layer-resolved DOS of central V layer in bct $Fe_3/V_5/(100)$ superlattice under hydrogenation.

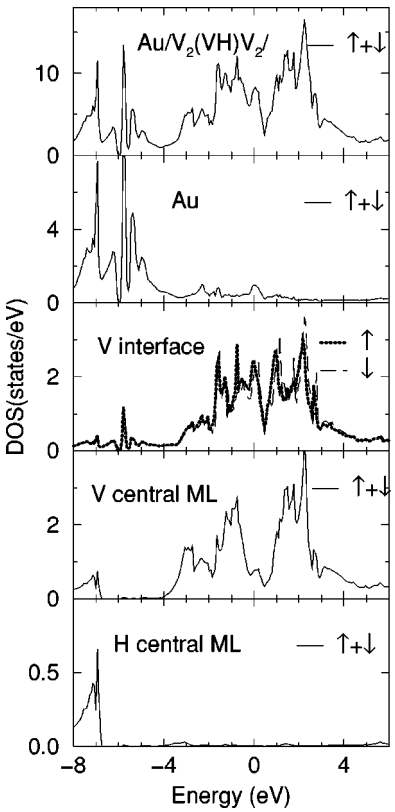

FIG. 8. The layer-resolved DOS of bct $Au/V_2(VH)V_2/(100)$ superlattice with the $a_{\parallel}$ of the bulk Fe and $c/a=1.1$ for the V layers.

moves versus hydrogen loading towards the Fermi level. The DOS at the Fermi level decreases monotonically from 1.7 to 0.1 when the hydrogen concentration c_H changes from 0 to 0.6 (see Fig. 7).

This low DOS at the Fermi level is able to explain unusual behavior of the Fe/V multilayers under hydrogen loading which was observed experimentally.[13,14] In more detail:

(1) The increase of the resistivity under hydrogenation was reported by Andersson and co-workers.[3] They postulated that this increase is exclusively associated with hydrogen as impurity atoms assuming that no major change in the electronic structure occurs. Influence of low DOS at the Fermi level will diminish the number of carriers in the V spacer but it will decrease also the probability of electron scattering. In the limit of very low DOS obtained here for high-hydrogen concentration, the resistivity has to increase without taking into account the additional impurity scattering.

(2) Oscillations of the IEC in metallic magnetic superlattices could be explained within the quantum well (QW) model through the oscillations of the energies of the electrons confined in the QW's formed by the magnetic slabs[15] or through the optical model with different electron refraction indexes for FM- and AF-coupled magnetic layers in superlattice.[26] Within a free electron model the oscillations of the IEC is governed by the dimensionless parameter $k_F L_0$, where $k_F=(2m\epsilon_F)^{1/2}$ is the Fermi momentum without transverse quantization and L_0 is the thickness of the nonmagnetic spacer. The period of the oscillations appears to be rather short: of the order of de Broglie wave length λ of electrons. One of the ways to overcome the discrepancy between the small period (about 2 Å) obtained in free-electron model and the long period (about 10 Å) observed in the experiment on Fe/V superlattices,[8] is to take into account the noncommensurability of the electron wavelength and the lattice constant. Usually the change of the spacer layer thickness can only occur by discrete values, which are a multiple of the lattice constant. As a result the observed period of oscillations period appears to be much larger than λ. In the case of the Fe/V superlattices the thickness of V spacer can be changed almost continiously under hydrogenation. So, short-range oscillations of the IEC can be observed as a transition from FM to AF coupling and vice versa. However, as we have seen from the calculations of the electronic structure, simultaneously with extention of the V spacer perpendicular to the superlattice plane direction, loading of the hydrogen leads to the decrease of the DOS at the Fermi level. This means the reduction of the amount of the electrons that are responsible for the AF IEC in the superlattice. Therefore, for a large hydrogen concentration the AF coupling has to disappear due to the diminution of the free-like electron's number in the V spacer.

The effect of the V DOS pinning is extremely sensitive to the details of the chemical structure of the magnetic and nonmagnetic layers. If into the V spacer a relatively small amount of Ag or Au, which brings additional electrons to the V film is introduced, it can shift the valley in the DOS away from the Fermi level and therefore return to the AF IEC. Similar phenomena was observed by Ebels *et al.*[27] in the Co/Ru multilayers, when a small amount of Ag introduced in the Co layer was able to change by π the phase of the IEC. To check this hypothesis, we performed the calculations of the electronic structure for bct Au/V_5H superlattice which consists of a single Au ML and 5 V ML with hydrogen on the central V ML. The layer-resolved DOS for this system is displayed in Fig. 8. It is interesting to note that the interface

V layer shows a small magnetic moment of 0.2 μ_B due to interaction with Au layer. This is in agreement with observation of the weak magnetism of monolayers and multilayers of V on Au films by Beckmann and co-workers.[28]

At the Fermi level, for the central V layer, there is a peak because of the hybridization between V $3d$ and Au $5d$ states whereas at the interface V layer this peak is essentially higher. Therefore, in the neighborhood of the Au atoms the increase of the V-DOS at the Fermi level is larger and the short-range IEC oscillations after doping the V spacer with Au can reappear.

IV. CONCLUSIONS

Ab initio FP-LMTO calculations were performed for the description of the electronic and magnetic structures of the Fe/V superlattices with and without hydrogen in the V spacer. Lattice expansion and tetragonal distortion in the V layers caused by the lattice mismatch or hydrogen loading changes essentially the value of the magnetic moments of the Fe and V interface atoms but saturation magnetization, which is determined by both the Fe and the V interface moments depends very weakly on the V lattice constant. Although the value of the polarization at the V interface atoms can be changed several times by distortion, the V layer second from the Fe/V interface has a moment which does not exceed 0.05 μ_B even for bct structure with in-plane V lattice constant and $c/a=1.1$. Hydrogen loading in the V spacer leads to the decrease of both the interface magnetic moment on V atoms and of the DOS at the Fermi level. Low DOS can be one of the reasons for the increase of the superlattice resistivity under hydrogenation and for the disappearance of the AF IEC for large hydrogen concentration. Doping the V film with Au increases the DOS at the Fermi level and the AF IEC can reappear.

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