Induced spin polarization in V:Fe_nV_m superlattices and thin V films on Fe substrates

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The spin polarization at the (100) and (110) Fe/V interfaces is investigated using the tight-binding linear muffin-tin orbital method. For both Fe_nV_m superlattices and thin V_m films on Fe substrates we consider epitaxial growth of V with in-plane interatomic distance equal to that of Fe and out-of-plane interatomic distance fitted to recover the volume of V bulk. We obtain a short-range induced spin polarization in V, as well as reduced Fe polarization at the Fe/V interface. In Fe_nV_m superlattices, V couples always antiferromagnetically with Fe. For thin V films grown on Fe(100) the V polarization presents oscillations (layered antiferromagnetic configuration). The magnetic moments of V and Fe depend on the crystallographic orientation of the sample. Our results are compared with the existing experimental observations. [S0163-1829(99)03521-3]

I. INTRODUCTION

Metallic V is known to be nonmagnetic, but magnetic susceptibility measurements showed a magnetic response in V particles.[1] Several calculations in the 1970s[2,3] predicted that slight structural changes (relaxations, reduction in the coordination) may induce magnetic ordering in V systems. Nevertheless, later studies of magnetism in different V systems (V bulk, surface, and V overlayers on noble metals) did not get a clear answer to this question.[4,5] At that point the research work was concentrated on Fe-V systems, due to the fact that the hybridization between V and a strong magnetic element like Fe could induce magnetic ordering in V. Both neutron-diffraction studies[6] and first-principles calculations[7,8] displayed sizeable magnetization on V atoms in disordered FeV alloys. Also Korringa-Kohn-Rostoker Green-function (KKRGF) studies for V impurities in Fe[9,10] and adsorbate V atoms on Fe substrate[11] gave significant magnetization for V. This induced spin polarization of V has been also predicted for Fe/V interface systems by several theoretical works.[12–17]

Fe/V interfaces can be produced easily using different techniques like molecular beam epitaxy or sputtering.[18–26] These systems are quite interesting, not only from the fundamental point of view but also for their possible applications. The analysis of these Fe/V interfaces is delicate. Theoretical and experimental works concerning the same sample have led sometimes to contradictory results. Even among the different theoretical calculations as well as among the existing experimental studies one can see important discrepancies. Let us briefly summarize the state of the art for both the superlattices and the overlayers.

For Fe/V superlattices, all studies have found that V couples antiferromagnetically with the Fe interface and there exists an induced magnetization in V interface atoms due to Fe. Recent x-ray magnetic circular dichroism (XMCD) experiments by Tomaz *et al.*[18] and Schwickert *et al.*[19] pointed out that the magnetization of V decreases monotonically and slowly as going from the interface to inner layers of the V slab, and that this behavior seems to be independent on the orientation of the sample. These experimental data are in total contradiction with all previous theoretical studies about these Fe/V systems,[12–15] which indicate that the induced magnetization of V decays very quickly as increasing V thickness, and show that the magnetic profiles of these superlattices should depend on the epitaxial orientation.

In the case of V overlayers on Fe substrate, experimental works[23–25] have found evidence of a net magnetic moment at the V interface, which couples antiferromagnetically with Fe. Walker and Hopster[24] observed that the surface of a 2-ML V overlayer on Fe(100) is aligned parallel to the Fe interface, while Fuchs, Totland, and Landolt[25] found oscillatory behavior for thicker coverages (3–4 ML). On the contrary, Finazzi *et al.*[23] did not find this oscillation and showed that for different V coverages (1–25 ML) the V was always antiferromagnetically coupled with the Fe substrate, claiming that ''only the first interface V layer has magnetic alignment due to direct exchange interactions with the Fe surface atoms.'' The available theoretical calculations[13,16,17] about these samples predicted for a V ML on Fe(100) and induced magnetic moment antiparallel to Fe magnetization, but as they are relatively restricted to one ML of V (and only in the 100 orientation) they could not investigate this oscillatory behavior of the V overlayers which has been found experimentally.

From all these studies on Fe/V interfaces, it is clear that there exists an induced magnetization at V interface (values from $0.3\mu_B$ to $1.5\mu_B$) antiferromagnetically coupled with the Fe substrate, and a decrease (5–20%) in the magnetization at the Fe interface atoms. However, there remains a strong controversy in two points: (i) the short- or long-range induced spin polarization in V and (ii) the dependence of the magnetic profile of the Fe/V interfaces on the crystallographic orientation.

In order to clarify those points and also to investigate the oscillatory behavior of the V magnetic moments in V overlayers on Fe, it is neccesary to perform a systematic study of these Fe/V interface systems as a function of the V thickness, epitaxial orientation, and possible intermixing, within the same theoretical model. It is the aim of the present work to do such a systematic study by performing *ab initio* calculations of the magnetic behavior at Fe/V superlattices and thin V films deposited on Fe substrate by using the TBLMTO method. We have studied Fe_nV_m superlattices ($m=1-11$) simulating the experimental samples of Tomaz *et al.*[18], considering only ferromagnetic Fe-Fe exchange coupling between Fe_n slabs because Schwickert *et al.*[19] have shown only this coupling for this range of V thickness. For V overlayers on Fe we have calculated the magnetic moments at different V coverages (1–4 ML). In order to analyze the dependence of the magnetic behavior of these systems with the crystallographic orientation, we have performed calculations for two different faces, (100) and (110), in both the superlattices and the overlayers.

The paper is organized as follows: in Sec. II we briefly comment on the theoretical model. In Sec. III our results for the superlattices and thin V films on Fe are presented and discussed. The main conclusions of the present study are summarized at the end.

II. THEORETICAL MODEL

The calculations are performed using a scalar-relativistic version of the k-space TBLMTO method[27,28] with the atomic-sphere approximation. This method is based on the local spin-density approximation[29] of the density-functional theory.[30] We have taken Fe_nV_m superlattices and overlayers for $n \geqslant 5$ ML, but it turned out that the results were not affected by the Fe thickness, when we take five or more Fe layers. Therefore Fe_5V_m superlattices ($m=1-11$ ML) and Fe_5V_l overlayers ($l=1-4$ ML) have been finally considered in our work. The lattice parameters of both Fe ($a_{Fe}=5.29$ a.u.) and V ($a_V=5.61$ a.u.) bcc bulks have been obtained by total-energy minimization. Assuming pseudomorphic growth, the in-plane interatomic distance of V is chosen to be the same as the calculated lattice parameter of bcc Fe, whereas the V-V out-of-plane interatomic distance is determined according to the constant volume approximation. The Fe-V interface distance is chosen as the arithmetic mean value of the calculated Fe and V lattice parameters. The calculations are performed using an increasing number of k points, until final convergence is obtained for at least 135 k points in the irreducible Brillouin zone. In the case of thin V films on Fe we consider enough layers of empty spheres to assure that there is no interaction between the V surfaces of adjacent supercells[31] (five monolayers of empty spheres were enough).

For all V thicknesses, we have considered the ferromagnetic (FM) and the layered antiferromagnetic (AFM) configurations, with the parallel and antiparallel couplings between Fe and V at the interface. In Fe_5V_m superlattices, for V thickness $m=1,3$, we have also considered the in plane-AFM configuration, namely $c(2\times2)$. This magnetic solution has not been found and thus for higher V thickness it was not considered. For thin V films on Fe we have taken this $c(2\times2)$ configuration as a valid input in all cases.

III. RESULTS AND DISCUSSION

A. Fe_5V_m superlattices

The results obtained in the case of Fe_5V_m for $m=1,3,5,7,9,11$ show a short-range induced spin polarization in V for both the (100) and (110) crystallographic faces. In Fig. 1 we report the magnetic profiles for $m=1,3,5,7,9,11$. For $m=7,9,11$ the spin polarization at the third V layer starting from the Fe interface, as well as at inner V layers, is nearly zero (as it is the case at the central layer of Fe_5V_5: see Fig. 1).

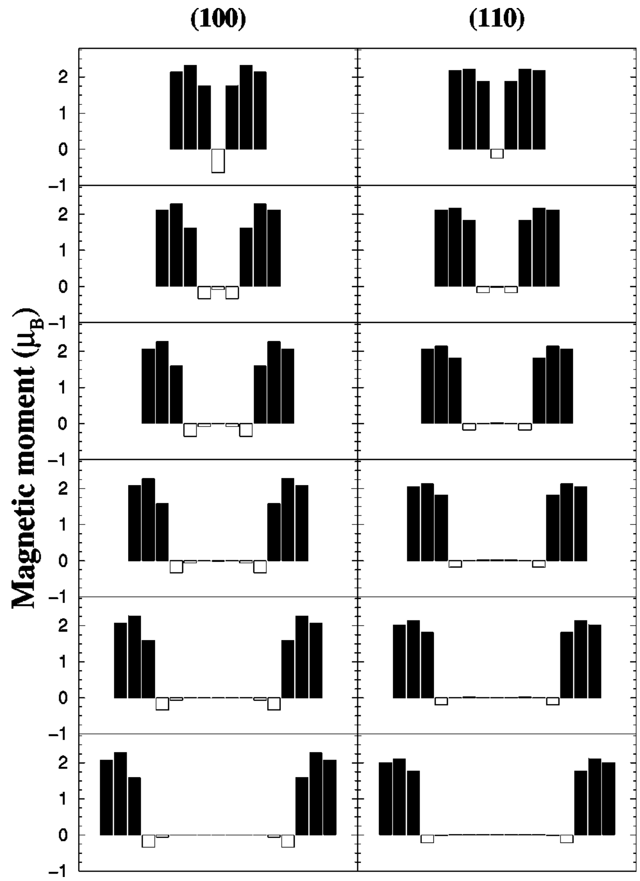

FIG. 1. Magnetic profiles (in units of μ_B) of Fe_5V_m ($m=1,3,5,7,9,11$) superlattices for (100) and (110) crystallographic orientations (left and right panels, respectively). Dark bars represent the values of the magnetic moments of Fe layers whereas open bars correspond to V.

In the left panel of Fig. 1, we show the results for the (100) orientation. We see that V is coupled antiferromagnetically with Fe for all thicknesses The induced spin polarization at the V interface has a sizeable value varying from $0.65\mu_B$ for Fe_5V_1 to $0.35\mu_B$ for $m \geqslant 3$. It is also clear the strong decrease of the V polarization as going from the interface to the inner layers of the V slab, the second V layer having less than $0.1\mu_B$. Another relevant trend is the reduction of the magnetization at the Fe interface atoms as compared to the bulk, while at inner Fe layers the magnetic moments slightly oscillate around the bulk value.

The right panel of Fig. 1 reports the magnetic profiles for the same V thicknesses as in the (100) crystallographic orientation. V at the interface couples antiferromagnetically with Fe, as in (100) superlattices, but the absolute values of the induced spin polarization are lower than those corresponding to the (100) orientation. The V moments are also strongly reduced as going from the interface to the inner V layers. In summary, we obtain a short-range induced spin polarization in V due to Fe for Fe/V superlattices grown on

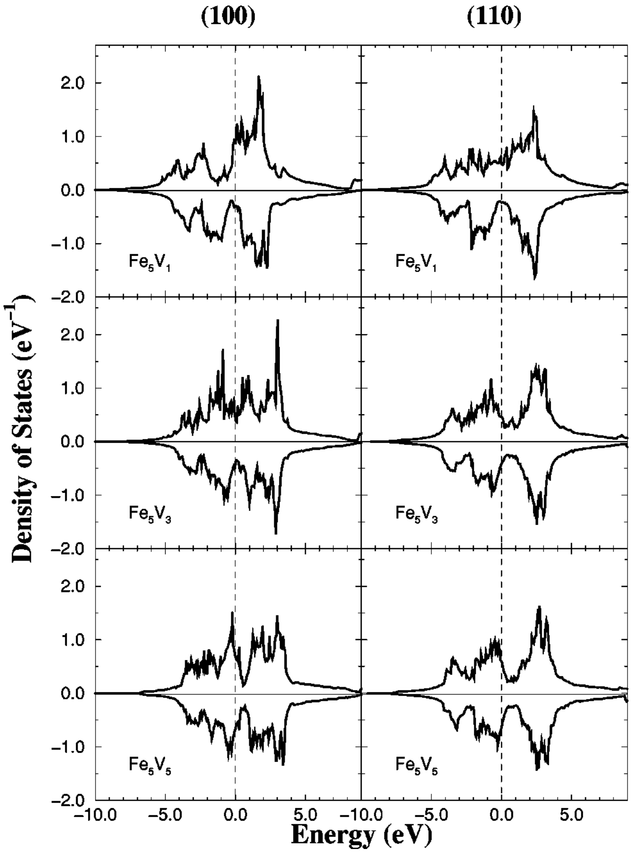

FIG. 2. Local density of electronic states (LDOS) at the central V layer of Fe_5V_m ($m=1,3,5$) superlattices for (100) and (110) crystallographic orientations (left and right panels, respectively). The vertical dashed line corresponds to the Fermi level.

both the (100) and (110) crystallographic orientations. For the (110) superlattices, the reduction of the Fe interface magnetization with respect to the bulk is less important than for the (100) superlattices (see Fig. 1).

We can understand the quantitative differences obtained for the two orientations by analyzing the different local chemical environment. In the (100) orientation, V has more Fe nearest neighbors at the interface than in the (110) orientation and thus larger Fe-V hybridization takes place. Therefore the induced magnetization in V due to Fe results larger in the (100) superlattices than in the (110) ones. For the same reason, Fe is more influenced by V in the (100) superlattices than in the (110) ones, leading to a stronger reduction in the Fe magnetization at the (100) interface than at the (110). All this is illustrated in Fig. 2, where we plot the local density of electronic states (LDOS) at the central V layer of the superlattices Fe_5V_m ($m=1,3,5$). The Fe-V hybridization effects are evident for Fe_5V_1, particularly through the splitting of the majority and minority spin components. The hybridization is more important for the occupied states than for the states above the Fermi level in both crystallographic orientations (due to the fact that the *d* band of Fe is more than half filled and the *d* band of V is less than half filled). The hybridization is also more important for the (100) than for the (110) and it reduces very fast as the V spacer increases. At Fe_5V_5 no spin splitting exists for the (110) orientation and a very small one is still appreciable for the (100) face. The convergence towards the V bulk limit is clear as increasing the number of V layers, but small differences between the LDOS of the two orientations remain as a consequence of the slightly distorted different V bulks for the (100) and the (110) faces.

Our calculations are in very good agreement with previous theoretical results that show a short-range polarization of V in Fe/V superlattices[12–15] and orientation dependence of the magnetic behavior. Our results, however, are not in good agreement with the x-ray magnetic circular dichroism (XMCD) measurements of Tomaz *et al.*[18] and Schwickert *et al.*[19] In these experiments the reduction in V magnetic moments as going away from the interface seems to be slower, supporting the existence of a longer range induced V polarization in Fe/V superlattices. They also find the same magnetic behavior independent of the crystallographic orientation, while we obtain measurable differences between the magnetization at the (100) and (110) interfaces. Concerning the absolute values, they obtain very large V magnetization. For the superlattice with one V monolayer they find more than twice our calculated value ($1.5\mu_B$ as compared to $0.65\mu_B$), and for all V thicknesses they find much higher values than in all previous works (in which V polarization at the interface never reach $1\mu_B$). In order to explain the discrepancies between theoretical and experimental results, the authors[18,19] pointed out that the presence of interdiffusion or intermixing at the Fe/V interface could be the origin of the enhancement of V magnetic moments. However, various experimental studies concerning the growth of Fe-V systems[21,22] have reported good epitaxial growth up to 7 ML (Ref. 22) and 9 ML (Ref. 21) of V and find that V deposition on the Fe(100) surface induces the formation of an abrupt interface without any diffusion in the Fe substrate. Even assuming the intermixing at the interface, experimental and theoretical works for alloys[6–8] and for V impurities in Fe (Refs. 9 and 10) never find such a large magnetization for V. We have also performed a calculation for the $Fe_3/Fe_{0.5}V_{0.5}/V_1$ superlattice (with Fe-V intermixing at the interface) and we did not find a high magnetic moment for V at the interface, in good agreement with a previous works by Coehoorn[14] for a similar system. Another disagreement between all theoretical works (including ours) and the cited XMCD experiments[18,19] is that no reduction of the Fe magnetization at the interface is observed, so that Fe atoms at the interface should have the same magnetization as in Fe bulk. Moreover, experimental measurements of Poulopoulos *et al.*[26] found this sizeable decrease in Fe magnetic moments at the Fe/V interface in good agreement with the theoretical results.

B. V overlayers on Fe

Concerning V thin films on Fe substrates, the experimental results[23–25] do not coincide in some significant trends. Walker and Hopster[24] reported an oscillatory behavior in the magnetization of V overlayers on Fe(100), finding that 1 ML of V couples antiferromagnetically with the Fe substrate while the surface of a 2-ML V film is coupled ferromagnetically with the Fe interface. These oscillations have been found also by Fuchs, Totland, and Landolt[25] but for different V coverages (3–4 ML of V). In contrast, Finazzi *et al.*[23]

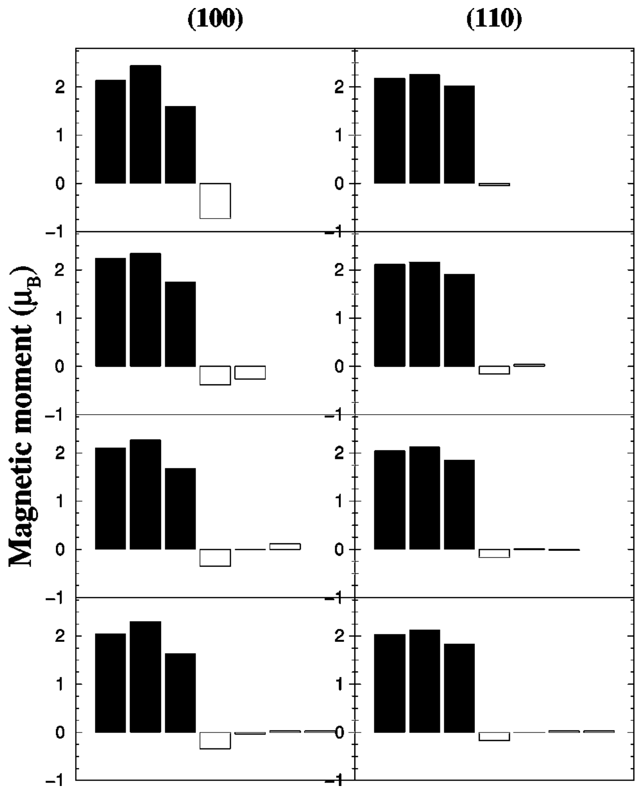

FIG. 3. Magnetic profiles (in units of μ_B) of V_m overlayers ($m=1,2,3,4$) on Fe(100) and Fe(110) (left and right panels, respectively); dark and open bars as in Fig. 1.

have observed antiferromagnetic coupling between V layers and the Fe substrate for all coverages investigated (1–25 ML), that is, no oscillations have been observed. All these experimental groups have obtained a fast decrease of the magnetization at the surface of the V films as increasing the V thickness, finding that for more than 4 or 5 ML, the V surface is nonmagnetic.

In Fig. 3 we present the magnetic profiles for 1, 2, 3, and 4 ML of V on Fe(100) and on Fe(110) obtained in our calculations. For the (100) crystallographic orientation (left panel of Fig. 3) the V interface has a significant magnetic moment induced by the Fe substrate independently of the V coverage. In the case of a single V monolayer on Fe(100) the magnetic moment of V is $\simeq 0.7\mu_B$. This value is in excellent agreement with previous *ab initio* calculations by Handschuh and Blügel,[16] and also with the experimental work of Walker and Hopster[24] in which they find that the magnetization of the V overlayer on Fe(100) must be less that $1\mu_B$. As V coverage increases, the V moments at the interface decrease up to a value of $\simeq 0.35\mu_B$ (see Fig. 2). This value is consistent with the experimental measurements at the V interface ($0.3\mu_B$) reported by Fuchs, Totland, and Landolt[25] for a similar system. We obtain the oscillatory behavior reported in part of the experiments[24,25] for 3 ML of V on Fe(100). Moreover, for coverages thicker than 4 ML, the V surface is nonmagnetic, in agreement with the experimental studies.[23–25] Finally we obtain a decrease in the magnetization of the Fe interface (about 20%) which is also in good qualitative agreement with the experiments.

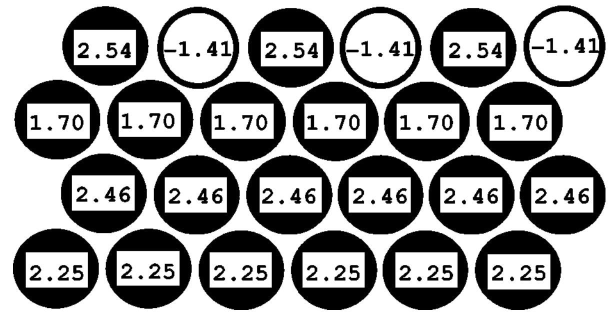

FIG. 4. Magnetic moments distribution at the ordered $Fe_{0.5}V_{0.5}$ surface alloy on Fe(100). Black and white circles correspond to Fe and V atoms, respectively.

In the case of the (110) crystallographic orientation (right panel of Fig. 3), our calculations give quite surprising but also interesting results. For all V coverages the local magnetic moment of V at the interface is antiparallel to that of the Fe substrate, but for a single V ML on Fe(110) we obtain a surprisingly small V magnetization ($0.05\mu_B$). We have tested, as input, the in-plane AFM configuration, namely $c(2\times 2)$. However, we could not converge it in our calculations. For 2, 3, and 4 ML, the magnetic behavior is similar to the one observed in the (100) orientation, with oscillations in the V magnetization as well as the short-range V polarization induced by the Fe substrate. As in the case of the superlattices, the V magnetization is larger for the (100) orientation than for the (110) and the reduction of the magnetization at the Fe interface is larger for (100) overlayers than for (110) ones. These trends can be explained, as for the superlattices, in terms of the different local chemical environment at the two orientations.

The effect of Fe-V intermixing on the magnetic properties of the overlayers has been also analyzed at the first stage of the growth in the (100) direction, that is for the simplest ordered surface alloy $Fe_5/Fe_{0.5}V_{0.5}$. The results, shown in Fig. 4, display a very enhanced magnetic moment in V. This result is in good agreement with *ab initio* KKRGF calculations[10,11] for V impurities in Fe(100) surface layer.

IV. SUMMARY

We have performed TBLMTO calculations of the electronic structure and magnetic properties of two different Fe/V interface systems: superlattices and V overlayers on Fe substrate. We have tested the dependence of the magnetism with the crystallographic orientation by studing (100) and (110) faces.

In Fe_nV_m superlattices, we find that the V interface has a sizeable magnetic moment coupled antiferromagnetically to the Fe substrate. We obtain a reduction in the magnetization of the Fe interface atoms as compared to the bulk. V magnetic moments decrease very quickly from the interface to inner layers of the V slab, so we conclude that there is an induced short-range polarization of V due to Fe substrate. The magnetic behavior of the system depends on the crystallographic orientation. The V interface in the (100) orientation is more magnetic than in the (110). At the same time, Fe interface shows smaller magnetic moments in the (100) orientation than in (110). This fact is explained in terms of the different local chemical environment of Fe and V for these two orientations. Our results are in very good agreement with previous theoretical studies[12,14] and some experimental data,[23] but not in good agreement with the experimental reports of Tomaz *et al.*[18] and Schwickert *et al.*[19] More specifically, the long-range polarization of the V spacer is at odd with the present result (and all previous *ab initio* calculations) displaying for Fe_nV_m superlattices a short-range polarization. One way to explain this long-range polarization is to introduce pinholes, i.e., an Fe bridge connecting two Fe slabs through V spacer. Up to now only semiempirical-type calculations were suitable to solve this type of problem, as performed by Uzdin and Demangeat[32] in the case of Fe/Cr/Fe trilayers, but the experiments did not find evidence of this kind of defects in these FeV samples.[33]

In the case of V thin films on Fe for (100) orientation, we find that 1 ML of V on Fe is aligned antiparallel with the Fe substrate, and has a measurable magnetic moment of $0.7\mu_B$ wich is in very good agreement with previous *ab initio* calculations[16] and also with experimental data.[24] We find also the oscillations in the V magnetization for 3 ML of V, in good qualitatively agrement with experimental data.[24,25] The magnetization at the V interface decreases as we consider thicker coverages of V to a limit of about $0.35\mu_B$, which coincides with the measurements of Fuchs, Totland, and Landolt.[25] For coverages thicker than 4 ML, the V surface presents no magnetic ordering. As in the superlattices we find a reduction in the Fe interface magnetization as compared to the bulk value. For (110) direction, our results seem to be more complicated. We have found a nearly nonmagnetic solution for a single V overlayer on Fe(110), but we think that this may not be the more stable configuration, being necessary the search of more complex magnetic configurations. This possibility has been also pointed out by Nawrath *et al.*[34] for ultrathin epitaxial Fe layers on V(110) in which they find that a 3-ML Fe film has no in-plane magnetization. For thicker coverages, the trends are similar to those obtained for the (100) orientation, but the values of the magnetic moments of V are smaller. The reduction of the magnetization at the Fe interface is also smaller. As in the superlattices this effect can be explained in terms of the different local chemical environment in the two orientations.

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