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# Magnetic reconstructions at the surface of the B2 FeV alloy

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**Abstract.** We present an *ab initio* study of the magnetic surface reconstructions of the B2 FeV alloy using a self-consistent tight-binding linearized muffin tin orbital method developed in the atomic spheres approximation. For (001) and (111), the surface reconstruction stabilizes configurations unstable in the bulk alloy. When Fe is at the (001) surface, a $c(2 \times 2)$ in-plane antiferromagnetic order is found to be the ground state with magnetic moments of $-2.32\mu_B$ and $2.27\mu_B$. A $p(1 \times 1)\downarrow$ ferromagnetic order is displayed in case of V toplayer with a magnetic moment of $-1.83\mu_B$. At the (111) surface, we obtain for Fe toplayer two solutions $p(1 \times 1)\uparrow$ and $p(2 \times 1)$. The configuration p(1×1)↑ is found to be the ground state with a magnetic moment per atom of $2.34\mu_B$. For V toplayer, only the $p(1 \times 1)\downarrow$ solution is obtained with a moment of $-0.84\mu_B$. In all cases, the Fe-V coupling is always antiparallel like in the bulk. Our results are discussed and compared to experiments.

**PACS.** 75.70.Rf Surface magnetism – 73.20.-r Electron states at surfaces and interfaces – 71.20.Be Transition metals and alloys

## 1 Introduction

V is a non-magnetic element in bulk whereas at the surface the situation is more controversial [1,2]. However it can be easily polarized in contact with a magnetic material.

The Fe-V systems (overlayers, superlattices, ...) have been the subject of numerous investigations both experimentally [3–16] as well as theoretically [8,19–26]. Most of these studies agree, in general, with a significant induced polarization on V at the Fe-V interface and an antiferromagnetic (AF) coupling between Fe and V is always reported at the interface.

However discrepancies in the range of the Fe induced polarization in the vanadium spacers, its shape reduction going away from the interface, a controversy on the occurring of an oscillating behavior between vanadium layers and the crystallographic orientation dependence of the magnetic behavior still remain up to now unsolved questions and more efforts are needed.

Sacchi *et al.* [6] by X-ray magnetic scattering (XRMS) measurements have obtained a sizeable induced magnetic moment on V at the Fe-V interface. They have shown that this moment is considerably diminished when one goes from a spacer of one monolayer (1 ML) to the case of more thicker samples in Fe/V(001) superlattices with an AF coupling at the Fe-V interface. X-ray magnetic circular dichroism (XMCD) study of Finazzi *et al.* [7] found at room temperature an AF coupling between V (1–25 ML) and Fe substrate at all coverages. Moreover, X-ray magnetic linear dichroism (XMLD) spectra of Schwickert *et al.* [8] displayed a sizeable magnetization on V in multilayered regime ($Fe_5/V_1$) and an AF coupling at the Fe-V interface. They obtain theoretical spectra of Fe and V in magnitude and shape in good agreement with their measurements.

Up to now the Fe-Fe magnetic coupling is supposed to be parallel. However recent experiments in magneto transport properties have underlined magnetic phenomena which contradict this such as giant magnetoresistance (GMR) [12–14], indicating AF coupling between successive Fe layers for appropriate V spacer thicknesses in V/Fe multilayers. Indeed, contrary to XMCD experiments of Finazzi *et al.* [7], magnetization measurements by mean of superconducting quantum interference device (SQUID) of Isberg *et al.* [12] have shown an AF coupling between successive Fe layers for vanadium thickness larger than 15 Å in Fe/V(110) superlattices. Similar coupling is also displayed in the Fe/V(001) superlattices by Granberg *et al.* [14] by mean of SQUID magnetometer, Labergerie *et al.* [5] *via* the magneto-optical Kerr effect (MOKE)

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and Poulopoulos *et al.* [15] using ferromagnetic resonance (FMR). However the range where this coupling occurs is somewhat different from an experiment to an other.

As it is revealed experimentally [17,18] the growth of vanadium atoms on the Fe(100) surface induces the formation of an abrupt interface without any diffusion in the iron substrate and a good epitaxial growth up to 6 or 7 ML [17] and 9 ML [18] of V is reported.

Izquierdo *et al.* [19] within tight-binding-linear-muffin-tin-orbital developed in the atomic sphere approximation (TB-LMTO-ASA) in the framework of the local spin density approach (LSDA) have recently shown that for the perfectly abrupt or mixed interfaces the long-range polarization does not exist in good agreement with the XRMS measurements of Sacchi *et al.* [6]. Also, Niklasson *et al.* [20] using Green's function technique (GFT) based on TB-LMTO within LSDA approximation have reported a spin induced polarization on V at the Fe-V interface. Their results show a fast decrease of the vanadium magnetic moment as going from the interface and a highly orientational dependence in good agreement with those of Sacchi *et al.* [6] and Izquierdo *et al.* [19]. Within TB-LMTO method with coherent potential approximation (CPA) Turek *et al.* [21] have investigated the iron-vanadium random alloy (001) surface. They have shown that the magnetic structure of the Fe-V random alloy (001) surface depends strongly on the alloy composition with, in general, a magnetic moment enhancement. Near the vanadium concentration of 0.8, a tendency to parallel alignment between Fe and V atoms is observed. On the other hand Ostanin *et al.* [27] within full-potential-linear-muffin-tin-orbitals (FP-LMTO) have shown that hydrogen induces a strong modification of the density of states (DOS) at the Fermi level so that this may explain the tuning of the oscillatory interlayer exchange coupling.

From all these theoretical studies a relevant point of general agreement is an induced magnetic polarization on V antiferromagnetically coupled with Fe at the Fe-V interface. Its magnetic moment value belong to the range of (0.3–1.5 $\mu_B$). However most of these previous calculations were restricted to systems with perfect (or almost perfect) abrupt interfaces. However when V is grown thermally on Fe substrates, or Fe on V substrates an ordered B2 FeV can form within a few layers. As a result the electronic structure and the magnetic map will be very different. It is therefore the purpose of the present communication to investigate about this surface terminated B2 FeV in order to verify the occurrence of magnetic reconstructions. These magnetic surface reconstruction may be of utmost interest for the explanation of the experimental results of the Fe/V multilayered systems. For example, what will be the V induced polarization when capped by one Fe layer or left at the open surface (Fe or V toplayer cases) and what effect the crystallographic orientation will have on the magnetic polarization? In the following we try to answer these questions, by considering V (or Fe) at the surface of the ordered B2 FeV alloy.

The FeV system is a substitutionnal alloy displaying a complete solubility at high temperature. Experimental phase diagram [28] and first principles study [29] have shown that the FeV alloy at the equiatomic composition acquires an ordered CsCl (B2)-type structure around 823 K [30]. Electronic structure calculations [21,31–34] and experimental [35–37] studies have been already obtained in the bulk phase. Different Fe-V couplings and magnetic moments were reported, from AF coupling [33,34] to those showing the FM coupling [32,35] or non-induced V polarization [31,36].

The aim of this work is therefore to study the magnetic surface reconstructions of the B2 FeV alloy. Section 2 is devoted to a brief report about the method used and numerical details. In Sections 3 and 4 we present and discuss our results concerning the (001) and (111) surfaces respectively. Finally in the last Section 5 we conclude our study.

## 2 Computational model

First-principles spin-polarized electronic structure calculations were performed using a scalar-relativistic version of the $k$-space TB-LMTO method [38–40] developed in the atomic spheres approximation (ASA). Based on the density functional theory formalism [41,42], both local spin density approach (LSDA) and generalized gradient approach (GGA) within the Von-Barth-Hedin [43] and the Langreth-Mehl-Hu [44] exchange-correlation term respectively, have been used. In this paper we focus mainly on GGA because, in general, it yields better results for the structural and magnetic properties of transition metals [45–47]. The LSDA calculations were carried out in order to compare the bulk results obtained in the framework of this study with previous theoretical results [21,31–34].

In order to find which magnetic reconstruction stabilizes the topsurface moment configurations, we have explored three well known high symmetry magnetic orders, namely the two ferromagnetic (FM) orders $p(1{\times}1)\uparrow$ and $p(1{\times}1)\downarrow$, and the $c(2{\times}2)$ in-plane antiferromagnetic (AF) order [45,48]. These configurations are only considered at the (001) surface. At the (111) surface a triangular symmetry is encountered so that magnetic moments are frustrated if one try a fixed antiparallel coupling. For this surface, in addition to the FM orders $p(1{\times}1)\uparrow$ and $p(1{\times}1)\downarrow$, we consider the $p(2{\times}1)$ order instead of the $c(2{\times}2)$ one [45]. The three magnetic configuration unit cells being different, it is misleading to compare the total energies in the first irreducible Brillouin zone (IBZ) of the $p(1{\times}1)$ or $c(2{\times}2)$ and $p(2{\times}1)$ configurations. Thereby we choose for the (001) surface the same unit cell [45], that is two inequivalent atoms per layer. Using the supercell technique, the surfaces are modeled by repeated slabs geometry [49]. It consists of a superposition of alternating metallic monolayers (ML) of Fe and V. Two successive slabs are separated by a sufficient number of layers of empty spheres (ES) in order to obtain well separated non-interacting slabs. We have also investigated if our surfaces are well modeled: we check if the central layer properties of the metallic part coincides with those of the bulk. We also discuss if one particular ground state is not affected by film thickness and we request that the magnetic moments at the surface toplayer should not vary over $10^{-2}\mu_{\rm B}$. Lattice parameter in our calculations is kept the same as that of the magnetic bulk determined by total energy minimization. Our calculations are performed using increasing $k$-points number until final convergence is obtained for a set of 648 $k$-points in the first IBZ. A reasonable thickness of the supercell is found to be 11 ML of metallic atoms and 7 ES for the (001) surface, and 9 ML and 9 ES for the (111) one. Let us mention that Meza-Aguilar *et al.* [50] have obtained, within the same approach, suitable results for the magnetic map at the surface of the Mn-Co ordered alloy.

Before computing the spin polarization of the (001) and (111) surfaces, we have determined the total energy and the magnetic structure versus lattice parameter of the bulk FeV alloy. The calculations are performed in the framework of both the LSDA approach within the von Barth-Hedin functional [43] and GGA approach within the Langreth-Mehl-Hu functional [44]. The total energy minimization present a parabolic dependence as function of the volume. The ground state is obtained for a lattice parameter of 5.45 a.u in GGA and 5.39 a.u in LSDA which are respectively 0.9% and 2.2% below the experimental value (5.50 a.u) [30]. For these lattice parameters, the Fe-V magnetic coupling is antiparallel. A transition from the FM coupling between the Fe and V atoms to the AF one occurs when going from low to large volume.

## 3 (001) surface

In this section we study, within the GGA approach, the magnetic map at the (001) crystallographic surface of the ordered B2 FeV alloy. First, we report the results for Fe toplayer and then those of V toplayer. In each case we consider the three magnetic configurations quoted above as input configuration in the self-consistent procedure.

For Fe toplayer three converged solutions are obtained that is $c(2\times2)$, $p(1\times1)\uparrow$ and $p(1\times1)\downarrow$. The in-plane AF order $c(2\times2)$ is found to be the ground state configuration with different local magnetization ($-2.32\mu_{\rm B}$, $2.26\mu_{\rm B}$) as consequence of the different magnetic environment at the surface (Fig. 1a). However, the two configurations $c(2\times2)$ and $p(1\times1)\uparrow$ are almost degenerated, the energy difference being 0.4 mRy. Then it is hard to decide which one is really the equilibrium configuration. An energy difference of 0.66 mRy has been obtained in LDA. Let us point out that the moments carried by the metallic central layer (mean magnetic moments of $1.14\mu_{\rm B}$ for Fe and $-0.28\mu_{\rm B}$ for V) for the $c(2\times2)$ configuration are close to those of bulk alloy ($1.04\mu_{\rm B}$, $-0.24\mu_{\rm B}$). We observe an increase of the Fe magnetic moments when going from inner layer to surface (S) contrary to V moments which follow a decrease behavior towards the subsurface (S–1). This induced decreasing polarization of V is due to the $c(2\times2)$ magnetic surface reconstruction at the Fe surface. As V couples normally antiferromagnetically with the Fe atoms the parallel orientation of half of the Fe surface atoms with them blocks the magnetic moments of the V subsurface atoms.

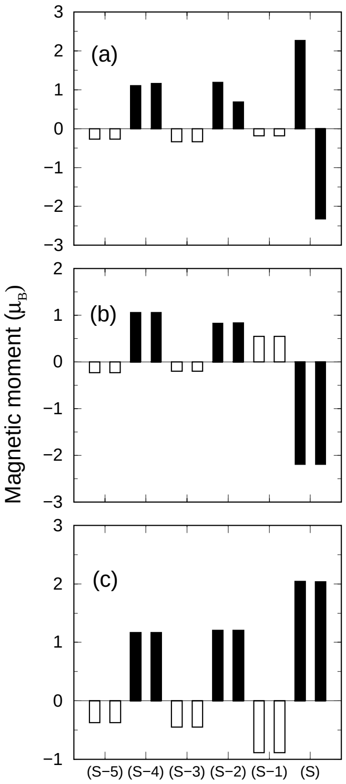

**Fig. 1.** Profiles of the magnetic moments for the three converged configurations $c(2\times2)$ (a), $p(1\times1)\downarrow$ (b) and $p(1\times1)\uparrow$ (c), at the (001) surface of the ordered B2 FeV alloy when Fe is toplayer (S). Black bars report the magnetic moments of Fe whereas white bars correspond to the V moments.

As it is established Fe successive layers oriented (001) are coupled ferromagnetically [13] except if the vanadium spacers exceed 12 ML for thin Fe layers (3 ML) where the coupling is AF [5,15]. Thus the decrease of the magnetic moment on one Fe site at (S–2) level seems not surprising although its in-plane nearest neighboring is not affected as a consequence of the $c(2\times2)$ surface configuration. To stabilize the surface configuration the outermost Fe atom with negative magnetic moment had to lower its next nearest Fe atom on layer (S–2).

For the metastable solution $p(1\times1)\downarrow$ (Fig. 1b) the magnetic moments carried by the surface toplayer ($-2.20\mu_{\rm B}$ per Fe atom) are slightly less enhanced than in the previous $c(2\times2)$ magnetic order. The bulk results are well recovered at the central layer ($1.07\mu_{\rm B}$, $-0.23\mu_{\rm B}$). A relevant point which seems *a priori* contradictory is encountered: a parallel coupling is found between adjacent Fe (S–2) and V (S–1) layers when this coupling remains (AF) elsewhere. We can understand the occurrence of this particular coupling by analyzing the polarization of the Fe layers surrounding that (S–1) vanadium layer. The V plane at (S–1) is sandwiched between two iron layers (S) and (S–2) coupled antiferromagnetically and displaying a large difference of polarization, hence V take the usual AF orientation with the Fe (S) plane carrying the highest value. We can also suspect an onset of non-collinear magnetism

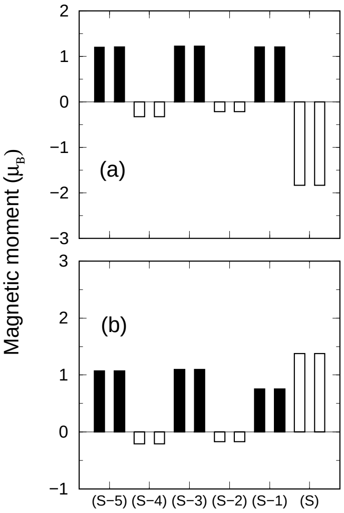

**Fig. 2.** Profiles of the magnetic moments for the two converged configurations $p(1\times1)\downarrow$ (a) and $p(1\times1)\uparrow$ (b), at the (001) surface of the ordered B2 FeV alloy when V is toplayer (S). Black bars report the magnetic moments of Fe whereas white bars correspond to the V moments.

as found by Freyss *et al.* [51] in Fe/Cr(001) superlattices using the tight-binding semi-empirical method.

The last converged solution $p(1\times1)\uparrow$ (Fig. 1c) shows a regular magnetic profile with a surface magnetic moment of $2.04\mu_B$. As we are going from inner to surface plane, for both Fe and V, an increasing polarization is obtained. This last solution $p(1\times1)\uparrow$ is characterized by a strong induced spin-polarization at the vanadium subsurface and a reduction of the magnetization at the Fe surface when compared to the two other converged solutions $c(2\times2)$ and $p(1\times1)\downarrow$.

We see also that the intensity of the spin-induced polarization in V subsurface depends strongly on its surface magnetic reconstructions. The regularity of the $p(1\times1)\uparrow$ configuration derives directly from the type of local magnetic environment surrounding an arbitrary atom in the same plane. In this configuration each atom has an identical magnetic neighborhood in the same plane. Evidently it is not the case in $c(2\times2)$ configuration, especially at the (S–2) plane.

In the second step we deal with the case of V toplayer. Only two solutions are obtained, namely $p(1\times1)\downarrow$ and $p(1\times1)\uparrow$ whereas for the $c(2\times2)$ input configuration, the self-consistent process converged to the $p(1\times1)\downarrow$ order. The $p(1\times1)\downarrow$ configuration plotted in Figure 2a is found to be the ground state with a high surface magnetic moment of $-1.83\mu_B$ per V atom. This configuration is characterized by a constant value of the Fe magnetic moment going from central layer towards the surface and its value is not significantly different from the bulk alloy. This ground state, compared to the $p(1\times1)\uparrow$ order for Fe toplayer, shows an unexpected magnetic profile: the moments of V (Fig. 2a) are not gradually enhanced although the Fe-V coupling remains AF at all interfaces.

The $p(1\times1)\uparrow$ configuration (Fig. 2b) also displays an unusual FM coupling between Fe at (S–1) and V at (S), due to the prefixed-spin-moment procedure. Similar behavior between Fe (S–2) and V (S–1) was obtained for the case of Fe toplayer in the $p(1\times1)\downarrow$ configuration. The central layer magnetic moments ($1.07\mu_B$, $-0.21\mu_B$) are in good agreement with those of the bulk alloy. The magnetic moments at the surface are very enhanced but remain less important than those of the ground state. For this configuration the Fe magnetization at the subsurface (Fig. 2b) is strongly reduced as compared to the inner layer or the bulk alloy. This can be understood by the fact that the vanadium surface in order to couple ferromagnetically with the Fe had to lower considerably the polarization of the Fe subsurface layer (frustration effect). The energy difference between $p(1\times1)\uparrow$ and $p(1\times1)\downarrow$ is 11 mRy.

To shed some light about the validity of some essential basic parameters, we have also performed calculations on which our model is based on, like the thickness effect of the slab and the number of $k$-points in the IBZ, on the total energy stability and the magnetic moments. A typical set of $k$-points such as ($k_x = 18$, $k_y = 18$ and $k_z = 1$) displays reasonable results since it leads to very close results as for another set of (18 18 2) , *i.e.* a difference of $10^{-4}$ $\mu_B$ for the magnetic moments and $10^{-6}$ Ry for the energy values. The increase of the thickness of the slab considered in our supercell has no effect neither on the $c(2\times2)$-like ground state nor on the surface magnetic moments of the three configurations studied.

The outermost layer of the (001) surface is characterized by different reconstructed magnetic configurations. Our calculations for this surface underline clearly the effect of a strong perturbation like the surface for both Fe and V. This effect is most important for the vanadium at the surface. As displayed in Figure 2a which represent the ground state a very important V moment with an AF coupling at the Fe-V interface is obtained. This result is in reasonable agreement with the XMCD results of Schwickert *et al.* [3] and Tomaz *et al.* [52] who found a sizeable induced polarization of $1.5\mu_B$ on V in $Fe_5V_1$ superlattices and an AF coupling at the Fe-V interface. On the other hand our calculations show a reduction of the Fe magnetization at the subsurface in disagreement with those authors [3,52] but in good agreement with all previous theoretical studies [19,20,23,24,26] and other experiments [5,15]. Moreover, the data obtained are in reasonable agreement with those of Vega *et al.* [24]. Their calculations display a strong influence of the surface as found in our calculations. They have obtained a high moment of $-0.83\mu_B$ on V for $Fe_3V_1$ film.

## 4 (111) surface

For the (111) surface of the ordered B2 FeV alloy and within the GGA approach we consider also two cases: Fe toplayer and V toplayer.

With Fe at the outermost layer of the surface, two converged solutions were obtained, namely $p(1\times1)\uparrow$ and $p(2\times1)$. The $p(1\times1)\downarrow$ as input configuration leads after the convergence process to the $p(1\times1)\uparrow$ solution which is found to be the surface ground state with a magnetic moment of $2.34\mu_{\rm B}$ per Fe atom. The Fe-V coupling remains AF like as the bulk. The moment carried by the vanadium subsurface layer ($-1.23\mu_{\rm B}$) is appreciably enhanced and is much stronger than that of the (001) subsurface for the same configuration. We can ascribe this to the stronger enhancement of the Fe moment at the (111) surface than at the (001) one resulting mainly from the number of coordination corresponding to each surface. Indeed, when Fe is at the toplayer of the (111) surface, it is surrounded by 3 nearest neighbors of V atoms and by 4 V atoms when it is at the toplayer of the (001) surface. The V neighborhood quenches the magnetic moment of Fe which decreases with the increasing number of V neighbors as discussed by Mirbt *et al.* [53] through calculations using GFT-TB-LMTO-ASA method together with LSDA approximation. They reported on the Fe magnetic moment as a function of the number of nearest V atoms and obtained $\sim 2.3\mu_{\rm B}$ for 3 V atoms neighbors and $\sim 2.1\mu_{\rm B}$ for 4 V atoms neighbors as in the (111) and (001) surfaces, respectively. This comparison with the (001) surface can also be made for the magnetic profile of Fe and V. An important increase of their spin polarization (Fig. 3a) is displayed at the surface and at the subsurface layers. The V atoms have a preferential tendency to couple antiferromagnetically with the Fe layers, so that the $p(1{\times}1)\uparrow$ configuration (or $p(1{\times}1)\downarrow$ in case of V toplayer for both (001) and (111) surfaces) among the three considered seems to be the ideal compatible configuration with this coupling. The Fe magnetic moment at the surface ($2.34\mu_{\rm B}$) is smaller as that of the pure Fe (111) surface [20] ($2.92\mu_{\rm B}$) because of the partial cancellation by the V subsurface.

For the metastable solution $p(2{\times}1)$ (Fig. 3b), the local magnetic moments carried at the surface on the two inequivalent atoms are $2.21\mu_{\rm B}$ and $-2.23\mu_{\rm B}$ while the subsurface displays V magnetic moments of $0.19\mu_{\rm B}$ and $-0.47\mu_{\rm B}$. The solution really obtained is the $p(2{\times}1)p(2{\times}1)$ configuration, the subsurface being also characterized by the $p(2{\times}1)$ magnetic order. As input configuration we have started with the $p(2{\times}1)$ configuration at the surface and $p(1{\times}1)\uparrow$ at the subsurface. After the self-consistent process the convergence have led to the $p(2{\times}1)p(2{\times}1)$ solution (a spin flop has occurred at the V subsurface). A similar magnetization profile was also obtained by Amalou *et al.* [45] for the B2 FeCr alloy with Fe toplayer at the (111) surface.

For V toplayer, only the $p(1{\times}1)\downarrow$ solution is obtained. The magnetic moment at the surface layer is $-0.84\mu_{\rm B}$ per V atom (Fig. 3c). The moments at the central layer ($1.31\mu_{\rm B}$ for Fe and $-0.23\mu_{\rm B}$ for V) are reasonably close to the bulk alloy. In our calculation procedure, the three input prefixed spin-polarization orders $p(2{\times}1)$, $p(1{\times}1)\downarrow$, and $p(1{\times}1)\uparrow$ at the surface have all converged to a $p(1{\times}1)\downarrow$. This solution exhibits an AF coupling at all Fe-V interfaces similar to the bulk alloy. The magnetization increases for the vanadium layers as we are going from inner layer towards the surface while that of Fe decreases. Let us underline a relevant point which concern the strong induced polarization on V surface followed by a significant reduction of the magnetization at Fe subsurface ($0.79\mu_{\rm B}$). We see also that the vanadium layer at the (S–2) plane displays very small magnetic moment ($-0.08\mu_{\rm B}$). This is due to the fact that this vanadium layer is in contact with an Fe layer at subsurface which displays a smaller magnetic moment as compared to the bulk.

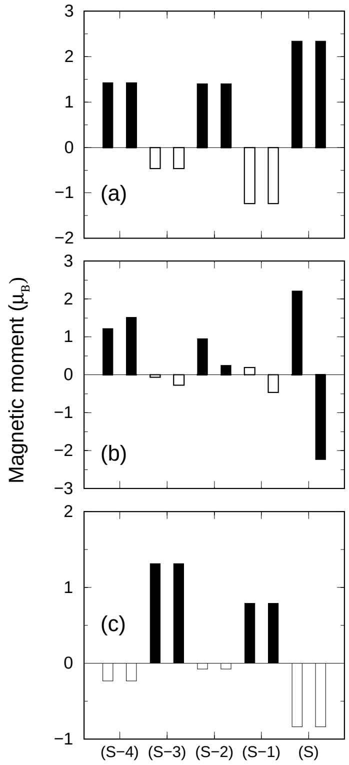

**Fig. 3.** Profiles of the magnetic moments for the two converged configurations $p(1{\times}1)\uparrow$ (a) and $p(2{\times}1)$ (b), at the (111) surface of the ordered B2 FeV alloy when Fe is toplayer (S). For V toplayer (S), only the $p(1{\times}1)\downarrow$ (c) solution is obtained. Black bars report the magnetic moments of Fe whereas white bars correspond to the V moments.

For the (111) orientation, the vanadium polarization is more important when localized at the subsurface than at the surface. The polarization of the V atoms is entirely induced by the hybridization with Fe since the magnetization of the vanadium layer is more enhanced when it is surrounded by iron layers (the case of the subsurface) than when it is at the more open (111) surface. An arbitrary V atom has more Fe nearest neighbors when lying at the subsurface than at the surface, so that due to a greater Fe-V hybridization, an important V induced magnetization by the Fe atoms occurs.

## 5 Summary

We have studied the surface magnetic configuration of the B2 FeV ordered alloy by mean of first-principles TB-LMTO-ASA method in the framework of the GGA approximation. We have investigated two surfaces, (001) and

(111) and for each surface we consider two cases: Fe at the toplayer and then V at the surface.

For the (001) surface with Fe toplayer, the configuration $c(2\times2)$ is shown to be, within our approximation, the ground state with magnetic moment of $2.27\mu_\mathrm{B}$ and $-2.32\mu_\mathrm{B}$. A magnetic reconstruction appears in the surface layer *i.e.* a configuration not present in the bulk alloy. A metastable state ($p(1\times1)\uparrow$ with magnetic moment of $2.04\mu_\mathrm{B}$ per Fe atom) and with small difference of energy with the ground state is also obtained. This solution presents the same magnetic configuration as in the bulk. However reservations concerning this statement are as follows. First, the calculated energy difference is at the verge of the validity of the ASA model. Second, we have neglected the dipole-barrier and third the magnetization of the central slab layer between $c(2\times2)$ and $p(1\times1)\uparrow$ differs non-negligibly.

For the V toplayer we obtain the configuration $p(1\times1)\downarrow$ as the ground state with a very high magnetic moment of $-1.83\mu_\mathrm{B}$ induced by the Fe atoms. A relevant point is that the surface effect is much more important for V and less for Fe. The V magnetization is much more enhanced at the surface than when it is at the subsurface.

In the case where Fe is a toplayer of the (111) surface, the $p(1\times1)\uparrow$ configuration is found to be the ground state with magnetic moments of $2.34\mu_\mathrm{B}$ per Fe atom. Moreover, an important induced polarization on V ($-1.23\mu_\mathrm{B}$) at the subsurface is displayed. For V toplayer the configuration $p(1\times1)\downarrow$ is the ground state with magnetic moments at the surface of $-0.84\mu_\mathrm{B}$ per V atom. The Fe magnetization at the subsurface ($0.79\mu_\mathrm{B}$ per Fe atom) is strongly reduced. The Fe-V coupling is AF at all interfaces for the (111) crystallographic surface.

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