Eur. Phys. J. B **48**, 249–254 (2005)
DOI: 10.1140/epjb/e2005-00388-7

THE EUROPEAN PHYSICAL JOURNAL B

From antiferromagnetic to ferromagnetic coupling for V adatoms on Co(001) substrates

T.A. Carrillo-Cázares[1], S. Meza-Aguilar[1,a], and C. Demangeat[2]

[1] Escuela de Ciencias Fisico-Matemáticas, Universidad Autónoma de Sinaloa, Bldv. de las Americas y Universitarios, Ciudad Universitaria, Culiacán Sinaloa, CP 80010, México
[2] Institut de Physique et Chimie des Matériaux de Strasbourg, 23 rue du Loess, 63034 Strasbourg Cedex 2, France

Received 27 April 2005 / Received in final form 6 September 2005
Published online 16 December 2005 –

Abstract. We discuss the polarization of V atoms on Co(001) substrates within density functional calculations. For sub-monolayer coverage the coupling between V and Co is clearly of antiferromagnetic type whereas it changes to ferromagnetic coupling in the case of a full V monolayer on Co(001). The results obtained in the case of a sub-monolayer coverage are in agreement with recent X-ray magnetic circular dichroism by Huttel et al. [Phys. Rev. B **68**, 174405 (2003)]. The transition from antiferromagnetic coupling (in the case of sub-monolayer coverage) to ferromagnetic coupling (for a full monolayer coverage) is discussed in terms of local coordination numbers and V-Co hybridization. Comparison with Cr and Mn coverages on Co(001) complicates the problem: i) submonolayer Cr coverage stabilizes the antiferromagnetic coupling between Cr and Co atoms (like for V on Co(001) whereas a Cr monolayer on Co presents in-plane antiferromagnetic coupling; ii) submonolayer Mn coverage stabilizes now the ferromagnetic coupling between Mn and Co whereas a Mn monolayer on Co(001) presents an in-plane antiferromagnetic coupling. Competition between Co induced magnetism and surface induced magnetism at V sites is discussed.

PACS. 75.70.Rf Surface magnetism – 68.47.De Metallic surfaces – 82.45.Mp Thin layers, films, monolayers, membranes – 75.70.-i Magnetic properties of thin films, surfaces, and interfaces

1 Introduction

Hattox et al. [1] showed that vanadium bulk undergoes a transition from a paramagnetic (P) to a ferromagnetic (F) configuration as the lattice parameter is increased. Akoh and Tasaki [2] found small V clusters to be magnetic. Also, Rau et al. [3] through electron-capture spectroscopy concluded to the existence of ferromagnetic order at the V(001) surface at odds with Full-potential linearized augmented plane wave (FLAPW) method of Ohnishi et al. [4]. Moruzzi and Marcus [5] have shown that, for bulk vanadium, antiferromagnetic (AF) structures appear more readily than ferromagnetic structures. Bouarab et al. [6]. have later shown that, also in the case of V slabs, the AF solution is more probable as the F one. The results of Ohnishi et al. [4] were corroborated by other ab initio calculations until the work of Bryk et al. [7] claiming a magnetic moment of $1.7\mu_B$ at the surface of V. Robles et al. [8] using a pseudopotential linear combination of atomic orbitals DFT method obtained similar results as those of Bryk et al. [7] but, within an all-electrons approach the surface magnetization remains zero.

Less controversial appears the case where vanadium is in contact with a ferromagnet as in Fe/V multilayered structures (see Vega et al. [9] for details). As discussed by Izquierdo et al. [10] the induced spin polarization of V slabs at the interface with Fe is of antiferromagnetic type. The induced spin polarization of V depends of the geometrical structure of the nanostructures considered. However, in all cases discussed (Fe/V superlattices or thin V overlayers on Fe substrates) the induced polarization is always short-ranged in agreement with recent XMCD results of Scherz et al. [11]. In the case of Co/V interfaces, Huttel et al. [12] within X-ray magnetic circular dichroism (XMCD) have extracted the vanadium and cobalt magnetic moments at the V/Co interfaces. The V moment decreases with increasing V coverage but the coupling between V and Co remains of antiferromagnetic type as long as the V coverage remains much less than a monolayer. The magnetic moment per V atom is about 2 μ_B whereas the magnetic moments at the surface of semi-infinite Co(001) decreases when the V coverage increases. For small V coverage a strong induced V moment is obtained. This strong magnetic moment on V atoms decreases when the V coverage increases, for two reasons. The first is related to the V-V distance. For very small

[a] e-mail: smeza@uas.uasnet.mx

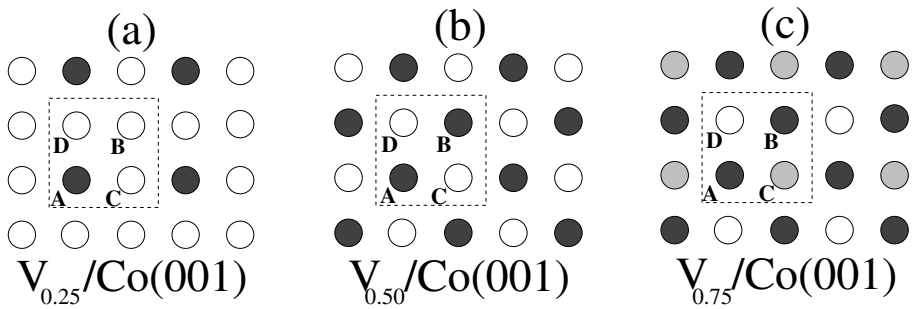

Fig. 1. Positions of the V atoms in the unit cell consisting of 4 sites labelled by A, B, C and D. For $V_{0.25}E_{0.75}$ only the site A is occupied by V atom, the other being empty. For $V_{0.5}E_{0.5}$ the V atoms are located at sites A and B whereas sites C and D are empty. Finally, for $V_{0.75}E_{0.25}$, A, B, and C sites are occupied by V atoms where site D is empty. Black and grey dots represent V atoms whereas white dots are empty spaces. The unit cell consists of 4 sites inside the dashed line.

V coverage this V-V distance remains large and the V atom looks like (apart hybridization with Co) an isolated V atom with high magnetic moment. For higher coverage the V-V distance decreases and the V atoms tend to look like in bulk vanadium i.e. presenting a non-magnetic behavior. The second reason of the decrease of the V moments versus coverage is connected to the fact (see Vega et al. [9]) that V tends to kill the magnetization in its surrounding i.e. when the V coverage increases the killing of the Co moment increases also. All these effects will be discussed in Section 3 of this paper. Our calculations present in this paper concern not only the submonolayer coverage of V on Co(001) as determined by Huttel et al. [12] but also a coverage by a thin film of V atoms.

We are not aware of any calculation on this system but, recently, Izquierdo and Demangeat [13] have reported on the magnetic configurations of a Co monolayer on Cr substrates. Following this particular calculation as well as those reported in Vega et al. [9] we discuss, in this paper, the magnetic polarization of V atoms on the face centered cubic (fcc) Co(001) substrate within TB-LMTO code. At this point we may ask why we are performing calculations on fcc Co slabs while bulk Co is hexagonal closed packed. The reason is that our purpose is to explain the XMCD results of Huttel et al. [12] who have evaporated V and Co on a cleaned Cu(001) surface. Thus, as discussed by Hong Li and BP Tonner [14] when the Co coverage on Cu(001) exceeds two monolayers, Co grows to a well-ordered fcc-(001) film via a layer-by-layer growth mode. The combination of low-energy electron diffraction and angle-resolved X-ray photoemission scattering shows that high quality fcc films of Co up to 20 monolayers thickness can be stabilized at room temperature by epitaxial growth [14].

We give a brief outline of the ab initio code used in Section 2, then we report in Section 3 the magnetic polarization obtained for various geometrical configurations of V adatoms on Co(001) substrates. The fcc Co substrate is modelled by a slab of 7 layers of Co atoms with V adatoms on both sides. This 9-layer slab is separated to the next one by 5 layers of empty spheres. Our model consist of various geometrical configurations, namely i) $V_{0.25}E_{0.75}$/Co(001) i.e. a repeated two dimensional cell containing one V atom and 3 empty spaces; ii) $V_{0.5}E_{0.5}$/Co(001) i.e. a cell with two V atoms and two empty spaces; iii) $V_{0.75}E_{0.25}$/Co(001) i.e. a cell with 3 V atoms and one empty space. These geometrical configurations are reported in Figure 1. Also, calculations for one, two and three V monolayers on Co(001) are reported. The geometrical configurations consist in these cases of a slab of 7 layers of Co with, respectively, one, two and three V layers at each side of the Co slab. Again, this slab (7 Co layers plus $2n$ ($n = 1$ to 3) V layers) is separated to the next one by 5 layers of empty spheres. The suitability of this model has been proven earlier by Khan [15]. The transition from antiferromagnetic coupling between V atoms and Co substrate, for submonolayer coverage to ferromagnetic coupling between V and Co for full monolayer coverage is rather hard to explain. In order to bring in some clue we have also performed calculations for Cr and Mn adatoms on Co(001).

Section 4 is devoted to the conclusion. The increase of the concentration of V atoms at the surface of semi-infinite Co substrate affects dramatically its induced polarization. This is linked to the fact that bulk vanadium is non-magnetic i.e. the induced V polarization is strongly reduced when the number of V atoms at the surface of Co(001) increases.

2 Methodology

The calculations are performed using a scalar relativistic version of the k space TB-LMTO method [17] with atomic sphere approximation. This method is based on the density functional theory [18]. We used, for Co, the lattice parameter for ferromagnetic phase which we obtained in previous work [19] for different functionals.

The overlayer system is modelled, using the repeated slab geometry [15] in which 7 layers of Co(001) with V atoms coverage at both sides of the slab and separated by five layers of empty spheres. These empty spheres are sufficient to prevent interaction between slabs [15] which is controlled throught vanishing dispersion in the direction perpendicular to the slab and vanishing charge in the central layer of the empty spheres. All atoms (Co, V) are located at ideal Co positions i.e. no structural minimization is considered. More precisely, the V atoms at the

Co/V interfaces are just replacing the Co atoms, one by one. This is indeed not entirely correct and it was shown by Tyer et al. [16] that relaxation may change the induced polarization in the case of Fe/W interfaces. We agree with this point of view but, in the present communication the situation is more complex i.e. we have considered various geometrical configurations and, in order to be fully consistent, we had to perform full relaxation in all cases. Nevertheless we have performed also a few calculations with an inwards relaxation of 5% in order to check its effect on the V-magnetic map. For low V coverage, we have restricted to a perfect two-dimensionnal ordered periodic lattice of vacancies which may be not the ground state configuration. A very perfect calculation should minimize the forces acting on all surfaces atoms. Moreover it should consider a Co-V exchange and check if this does not lead to lower total energy. The calculations are performed using an increasing number of k points until final convergence is obtained in the irreducible Brillouin Zone. This is discussed in details in the Ph.D. thesis of Meza-Aguilar [20]. The description for the V_xE_{1-x}/Co(001), (where E is the empty sphere and x is equal to 0.25, 0.50 and 0.75) needs calculations with 4 inequivalent atoms per layer. In the case of the nV/Co(001) (where n is 1, 2 and 3) we have restricted to 2 inequivalent atoms per plane. This permits us to consider both ferromagnetic and all in-plane antiferromagnetic configurations. Exchange correlation functional of Perdew-Wang-91 [21] was used to perform all calculations.

3 Results

The aim of the present paper is twofold: i) the first part is devoted to a a numerical determination of the magnetic map of V adatoms on Co(001) in the submonolayer coverage in order to explain the results of Huttel et al.; ii) the second part is to determine the magnetic polarization of a few V monolayers on Co(001). For submonolayer V coverage the results obtained are in agreement with the XMCD results of Huttel et al. [12]. However it is striking to see a complete reversal of the V induced polarization for a full V coverage. In order to get some clarification of this change of polarization we have also performed similar calculations for Cr and Mn coverages.

In this section we report the magnetic polarization of various concentrations of V atoms on Co(001). Without doing any calculation we can say, following the fact that isolated V atom presents a sizeable magnetic moment whereas bulk vanadium is non-magnetic, that a submonolayer V coverage of semi-infinite Co(001) will necessarily present a strong V moment whereas, for films of V on Co(001) the induced magnetization will be small.

We present first, results concerning a sub-monolayer V coverage whose geometrical configurations are reported in Figure 1. In this Figure 1 only the surface layer containing V atoms is reported. For all V concentrations, from 0.25 till 0.75 a sizeable magnetic moment per V atom is always obtained. Moreover an antiferromagnetic polarization between the V and the Co atoms is predominantly obtained and the results are reported in Table 1. Let us comment these results. First, when the V concentration is low (0.25 monolayer) the magnetic moment on each V atom is as high as 2.72 μ_B whereas the magnetic moments of the surface Co atoms (in contact with V) are slightly diminished. This can be explained from the fact that the V atoms are nearly isolated (at least far from another V atom) and the Co atoms, being ferromagnetic, are inducing magnetization on the V atoms. Second, when the concentration is 0.5 monolayer with the geometrical configuration displayed in Figure 1b, the V-V distance is diminished. This leads to two effects: i) a small decrease of the V magnetic moment and ii) a small decrease of the Co magnetic moment. For a V concentration of 0.75 monolayer a strong decrease of the V moments is observed. More precisely the V atoms at next nearest neighbor positions, i.e. at A and B, display a sizeable decrease of their magnetic moments as compared to the 0.5 monolayer coverage. Moreover the third V atom at C position (in the unit cell shown in Fig. 1c) presents a ferromagnetic coupling with the Co substrate and an antiferromagnetic coupling with its nearest neighboring V atoms at A and B positions. This last point is in agreement with what is known concerning the onset of magnetism in bulk vanadium when the lattice parameter is increased [5].

Table 1. Magnetic moments (in μ_B) for 3 concentrations of V atoms on Co(001) slabs: a) $V_{0.25}E_{0.75}$ corresponding to configuration a) of Figure 1; $V_{0.50}E_{0.50}$ corresponding to configuration b) of Figure 1. Magnetic moments on the V atoms on sites A and B are equal, due to symmetry; and c) $V_{0.75}E_{0.25}$ on Co(001) fcc substrate. For c) the magnetic moments on the V atoms are found inequivalent. A, B, C, and D are the 4 sites of the unit cell; E is the empty space. Co4 (Co1) atoms are in the interface layer with V atoms (in the center of the slab).

(a) $V_{0.25}$ Atom		(b) $V_{0.50}$ Atom		(c) $V_{0.75}$ Atom	
Va	−2.72	Va	−2.57	Va	−1.67
Eb	−0.01	Vb	−2.57	Vb	−1.67
Ec	−0.07	Ec	−0.12	Vc	0.86
Ed	−0.07	Ed	−0.12	Ed	0.11
Co4a	1.54		1.30		1.32
Co4b	1.54		1.30		1.32
Co4c	1.54		1.30		1.32
Co4d	1.54		1.30		1.32
Co3a	1.68		1.69		1.75
Co3b	1.64		1.69		1.75
Co3c	1.65		1.68		1.73
Co3d	1.65		1.68		1.73
Co2a	1.77		1.75		1.70
Co2b	1.77		1.75		1.70
Co2c	1.77		1.75		1.70
Co2d	1.77		1.75		1.70
Co1a	1.74		1.73		1.71
Co1b	1.74		1.73		1.71
Co1c	1.74		1.74		1.70
Co1d	1.74		1.74		1.70

Table 2. Magnetic polarization (in μ_B) of one (a), two (b) and three (c) monolayers of V on Co(001) fcc substrate. Here, due to periodicity we have restricted to unit cell of 2 inequivalent atoms in order to consider, not only the simple ferromagnetic or antiferromagnetic coupling between V and Co but also a possible in-plane antiferromagnetic configuration in the V plane. The Co4 (Co1) atoms are in the interface with the V overlayer (in the center of the slab).

	(a) V/Co(001)	(b) 2V/Co(001)	(c) 3V/Co(001)
Atom			
V3a			0.04
V3b			0.04
V2a		−0.06	−0.03
V2b		−0.06	−0.03
V1a	0.47	−0.20	−0.18
V1b	0.47	−0.20	−0.18
Co4a	1.17	1.15	1.22
Co4b	1.17	1.15	1.22
Co3a	1.79	1.75	1.73
Co3b	1.79	1.75	1.73
Co2a	1.69	1.70	1.69
Co2b	1.69	1.70	1.69
Co1a	1.70	1.71	1.70
Co1b	1.70	1.71	1.70

In order to be complete we have also considered higher V coverages in order to see more precisely the effect of the V-V distance on the magnetic moments of the V atoms. For one, two and three V layers on Co(001) the results are reported in Table 2 whereas the mean magnetic moment for V atoms in terms of the V coverage is reported in Figure 2. For a complete V monolayer coverage a drastic modification of the distribution of the V magnetic moments is found. For one V monolayer on Co(001) we have considered an unit cell of successively one and two inequivalent V atoms in order to see if complex magnetic configuration could be stabilized. For one inequivalent V atom, per plane, both layered ferromagnetic or antiferromagnetic couplings can be obtained whereas for two inequivalent V atoms in-plane antiferromagnetic configuration can also being obtained. For unit cells with one or two V atoms, in the case of a V monolayer on Co(001), the self-consistent procedure converges to the results reported in Table 2 i.e. a ferromagnetic coupling between surface V atoms and subsurface Co atoms. No in-plane antiferromagnetic coupling in the V monolayer was obtained.

This magnetic configuration is very different from that obtained for submonolayer coverages where essentially an antiferromagnetic coupling between V and Co was calculated and observed experimentally by Huttel et al. [12] The reason of this modification of the V-Co coupling remains rather obscure. Of course the decrease of the magnetic moment per V atom can be attributed to the fact that each V atom is now surrounded by 4 other V atoms at nearest neighboring positions. If we remember that a V atom surrounded by 8 nearest neighboring V atoms do not present magnetic moment it is clear that the increase of the number of V atoms around a given one may

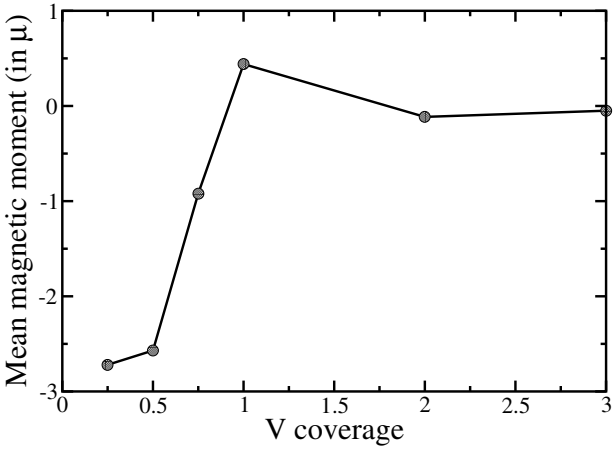

Fig. 2. Mean magnetic moment per V atom (in μ_B) in function of the V coverage. A drastic change of the direction of polarization is observed at full V coverage.

lead to some killing of their magnetic moment. For submonolayer V coverages the magnetic moment per V atom looks nearly like atomic vanadium with atomic-like moment whose value is not too disturbed by the Co neighbors. For a complete V monolayer the distances between the V atoms look more like in the bulk i.e. with a small (or negligible) moment like in the bulk case. Now, the effect of Co is to polarize the V atoms. Contrary to what happens at the Fe/V interfaces (the Fe-V coupling is of antiferromagnetic type) here the coupling between Co and V is of ferromagnetic type. For one V monolayer on Co(001) the coupling is of ferromagnetic type whereas for two and more V layers on Co(001) the coupling between V and Co, at the Co-V interface at least, is of antiferromagnetic type like in the case of the submonolayer regime.

When we go from one to two and three V monolayers the Co-V coupling changes from ferromagnetic to antiferromagnetic. Moreover only the V atoms at the nearest neighbor distances are likely to be polarized. Like at the Fe-V interface, the V polarization at the Co-V interface remains short-ranged.

Our results are in agreement with the XMCD results of Huttel et al. [12] for both V and Co. For $V_{0.25}$ coverage we obtained an AF polarization between V and Co with V = -2.72 μ_B and Co = 1.54 μ_B as compared to -1.9 μ_B and 1.65 μ_B for Huttel et al. For a monolayer concentration of 0.5ML for V we obtain, for V, a moment of -2.57 μ_B and for Co a moment of 1.30 μ_B as compared to -1.8 μ_B and 1.5 μ_B for Huttel et al. [12] It is well known that a fully self-consistent calculation should consider the effect of a small relaxation (small because Co and V belong to the same transition-metal series) on the V-magnetic map. Moreover it is necessary to see if the calculation without relaxation does not produce fortitious agreement with the available experimental results. In order to check this point we have performed calculations for a $V_{0.25}$ coverage and for a complete V overlayer on fcc Co(001), with an inwards relaxation of 5%. For the $V_{0.25}$ coverage the magnetic moment on V decreases from

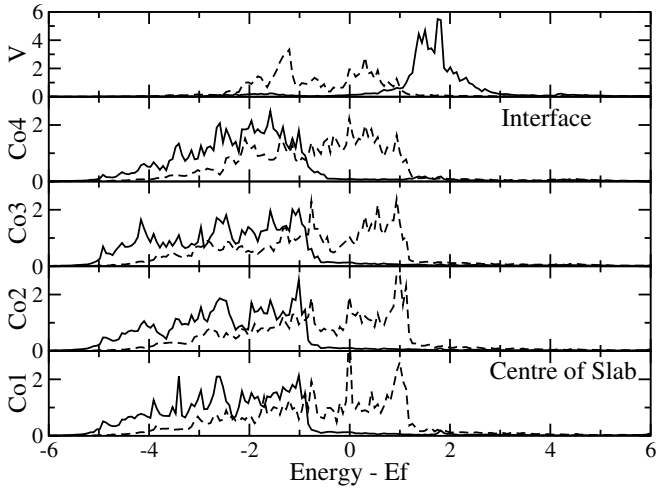

Fig. 3. Layer-resolved density of states (in states/eV) for the $V_{0.25}$ on Co(001) fcc system, separated in spin up (full line) and spin down (dashed line) bands.

$-2.72\ \mu_B$ to $-2.50\ \mu_B$ and is therefore in better agreement with the experimental result of $-1.9\ \mu_B$ [12]. For the full V-coverage the V-magnetic moment increases slightly from $0.47\ \mu_B$ to $0.50\ \mu_B$. Consequently relaxation effect has, at least for the present system, only marginal effect on the magnetic map.

Huttel et al. have proposed a simple model based on the position of the centroids of the spin-up and spin-down bands of Co and V. This model follows a proposal by Tyer et al. [16]. However, this simple model cannot explain the transition from antiferromagnetic couplings between V and Co (for submonolayer V coverage) to ferromagnetic coupling between V and Co (for a complete V monolayer on Co). More precisely, in the case of Fe/W multilayers, the polarization at the Fe-W interface is always antiferromagnetic whereas for a V monolayer on Co(001) the coupling at the interface is of ferromagnetic type. This coupling (between V and Co) is however of antiferromagnetic type when the V coverage is equal to 2 and 3 V monolayers or when the V coverage is less than a monolayer. For a V coverage less than a monolayer (0.25 for example), the width of the V local band is reduced because of the strong decrease of V-V bonds. The width of the V LDOS is much more reduced for spin-up because the centroid of the band is above Fermi-level E_F so that it has almost no hybridization with the Co-up spin bands located almost entirely below E_F. The V-up spin bands being almost entirely above E_F the number of V-up spin electrons remains small. Most of the electrons are therefore located in the V-down spin bands so that the V-Co polarization is of antiferromagnetic type (see Fig. 3).

In order to shed more light on these various couplings we have also investigated the magnetic polarization of Cr and Mn atoms adsorbed on Co(001). Table 3 compares the results obtained for $X_{0.25}E_{0.75}$ (X = V, Cr, Mn) on Co(001). For Cr and Mn coverages two solutions are obtained. The magnetic coupling, in the ground states is antiferromagnetic (like in the case of V) for Cr but it is ferromagnetic for Mn. Also a full monolayer coverage of Cr and Mn were investigated: for both type of atoms an in-plane antiferromagnetic coupling was obtained (Tab. 4). This last behavior may be reminiscent from the antiferromagnetic like coupling found in Cr and Mn bulks.

Table 3. Magnetic moments (in μ_B) for $V_{0.25}$, $Cr_{0.25}$ and $Mn_{0.25}$ on Co(001) fcc substrate for GGA-PW91 approximation using 4 inequivalent atoms per layer (similar to part a) of Tab. 1). For Cr and Mn coverage 2 solutions are obtained. The ground state is noted 0.00 and the difference of total energy between the metastable solution and the ground state is noted DTEC (in mRy).

System	$V_{0.25}$	$Cr_{0.25}$		$Mn_{0.25}$	
DTEC	0.00	0.00	98	36	0.00
Atom					
Xa	−2.72	−3.91	3.76	−4.24	4.06
Eb	−0.01	−0.01	−0.00	0.00	−0.01
Ec	−0.07	−0.06	0.01	−0.04	−0.01
Ed	−0.07	−0.06	0.01	−0.04	−0.01
Co4a	1.54	1.63	1.71	1.50	1.67
Co4b	1.54	1.63	1.71	1.50	1.67
Co4c	1.54	1.63	1.71	1.50	1.67
Co4d	1.54	1.63	1.71	1.50	1.67
Co3a	1.68	1.65	1.66	1.65	1.66
Co3b	1.64	1.65	1.66	1.65	1.66
Co3c	1.65	1.62	1.64	1.62	1.62
Co3d	1.65	1.67	1.70	1.68	1.66
Co2a	1.77	1.72	1.71	1.75	1.75
Co2b	1.77	1.72	1.71	1.75	1.75
Co2c	1.77	1.72	1.71	1.75	1.75
Co2d	1.77	1.72	1.71	1.75	1.75
Co1a	1.74	1.68	1.66	1.71	1.72
Co1b	1.74	1.70	1.66	1.71	1.72
Co1c	1.74	1.70	1.72	1.71	1.70
Co1d	1.74	1.70	1.73	1.71	1.72

From the previous calculations and comments we deduce the following explanation. For nearly "isolated" V adatom on Co(001) i.e. $V_{0.25}E_{0.75}$ the coupling of the V atom with nearest Co atom is of antiferromagnetic type (see the LDOS of Fig. 3). For the $V_{0.5}E_{0.5}$ configuration the V adatoms are at next nearest neighbor positions so that their coupling remains of ferromagnetic type as it should be. Moreover the V-Co couplings remain of antiferromagnetic type. When the V coverage is increased to $V_{0.75}E_{0.25}$ the situation is now completely different: there exist now V atoms at nearest neighboring positions. They should be of antiferromagnetic type. Finally for a complete V monolayer coverage each V atoms is now surrounded by 4 other V atoms at nearest neighbor positions. This certainly leads to a nearly killing of the magnetic moments. The remaining V moments (see Tab. 2) arise from the induced polarization through the Co substrate.

4 Conclusion

In this paper we reported results concerning the V polarization of V atoms deposited on Co(001) substrates. For submonolayer coverages the size of the V moments appear considerable and the coupling between V and Co

Table 4. Magnetic polarization (in μ_B) for V ML (a), Cr ML (b) and Mn ML (c) on Co(001) fcc substrate. Here, due to periodicity we have restricted to unit cell of 2 inequivalent atoms in order to consider, not only the simple ferromagnetic or antiferromagnetic coupling between V and Co but also a possible in-plane antiferromagnetic configuration in the V plane. The Co4 (Co1) atoms are in the interface with the V, Cr and Mn overlayer (in the center of the slab); Xa and Xb are the surface atoms.

Atom	(a) V/Co(001)	(b) Cr/Co(001)	(c) Mn/Co(001)
Xa	0.47	2.94	3.22
Xb	0.47	−2.87	−3.51
Co4a	1.17	1.36	1.15
Co4b	1.17	1.36	1.14
Co3a	1.79	1.76	1.75
Co3b	1.79	1.74	1.79
Co2b	1.69	1.69	1.71
Co2b	1.69	1.69	1.71
Co1a	1.70	1.72	1.71
Co1b	1.70	1.64	1.71

is of antiferromagnetic type. Our results are in agreement with those of Huttel et al. [12] Our model calculation gives the good trend of the magnetic polarization. Moreover the plotting of the LDOS shows clearly that the simple model proposed by Huttel et al. can explain this behavior. We have also performed calculations for full V coverages. For this geometry the size of the V moments is considerably lower whereas the V-Co coupling depends on the thickness of the V overlayers. Contrary to submonolayer coverage, no simple explanation arising from the LDOS plotting was obtained. More dramatically, the result concerning the induced V-polarization is opposite to that obtained by Tyer et al. [16] for W-polarization. Calculations concerning Cr and Mn overlayers does not lead to a more deep insight of this "a little bit strange" variation of the V polarization at the V-Co interface.

Very interesting comments by Yves Huttel are gratefully acknowledged. Institut de Physique et Chimie des Matériaux de Strasbourg is Unité Mixte de recherche 7504 (CNRS-ECPM-ULP).

References

1. T.M. Hattox, J.B. Conklin, J.C. Slater, J.C. Trickey, J. Phys. Chem. Sol. **34**, 1627 (1973)
2. H. Akoh, A. Tasaki, J. Phys. Soc. Jpn **42**, 791 (1977)
3. C. Rau, C. Schneider, G. Xing, G. Jamison, Phys. Rev. Lett. **57**, 3221 (1986)
4. S. Ohnishi, C.L. Fu, A.J. Freeman, J. Magn. Magn. Mat. **50**, 161 (1985)
5. V.L. Moruzzi, P.M. Marcus, Phys. Rev. B **42**, 8361 (1990)
6. S. Bouarab, H. Nait-Laziz, C. Demangeat, A. Mokrani, H. Dreyssé, Phys. Rev. B **46**, 889 (1992)
7. T. Bryk, D.M. Bylander, L. Kleinman, Phys. Rev. B **61**, R3780 (2000)
8. R. Robles, J. Izquierdo, A. Vega, L.C. Balbás, Phys. Rev. B **63**, 172406 (2001)
9. A. Vega, J.C. Parlebas, C. Demangeat, Handbook of Magnetic Materials, edited by K.H.J. Buschow (Elsevier Science B. V., 2003), Vol. 15, 199
10. J. Izquierdo, A. Vega, O. Elmouhssine, H. Dreyssé, C. Demangeat, Phys. Rev. B **59**, 14510 (1999)
11. A. Scherz, P. Poulopoulos, H. Wende, G. Ceballos, K. Baberschke, J. Appl. Phys. **91**, 8760 (2002); A. Scherz, H. Wende, K. Baberschke, K. Minár, D. Benea, H. Ebert, Phys. Rev. B **66**, 184401 (2002)
12. Y. Huttel, G. van der Laan, T.K. Johal, N.D. Telling, P. Bencok, Phys. Rev. B **68**, 174405 (2003)
13. J. Izquierdo, C. Demangeat, Phys. Rev. B **62**, 12287 (2000)
14. Hong Li, B.P. Tonner, Surf. Sci. **237**, 141 (1990)
15. M.A. Khan, J. Phys. Soc. Jpn **62**, 1682 (1993)
16. R. Tyer, G. van der Laan, W.M. Temmerman, Z. Szotek, H. Ebert, Phys. Rev. B **67**, 104409 (2003)
17. O.K. Andersen, O. Jepsen, Phys. Rev. Lett. **53**, 2571 (1984); O.K. Andersen, Z. Pawlowska, O. Jepsen, Phys. Rev. B **34**, 5253 (1986). The standard TB-LMTO-ASA code (version 47) developed by O.K. Andersen et al. at M.P.I. Stuttgart, Germany, was used
18. P. Hohenberg, W. Kohn, Phys. Rev. **136**, B864 (1964); W. Kohn, L.J. Sham, Phys. Rev. **140**, A1133 (1965)
19. B. M'Passi-Mabiala, S. Meza-Aguilar, C. Demangeat, Surface Science **518**, 104 (2002)
20. S. Meza-Aguilar, Ph.D. thesis, Strasbourg, France, 2000, unpublished
21. J.P. Perdew, J.A. Chevary, S.H. Vosko, K.A. Jackson, M.R. Pederson, D.J. Singh, C. Fiolhais, Phys. Rev. B **46**, 6671 (1992); J.P. Perdew, Y. Wang, Phys. Rev. B **45**, 13244 (1992)