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► To cite this version:

T. A. Carrillo-Cazares, S. Meza-Aguilar, C. Demangeat. Antiferromagnetism at V/Co(001) interfaces. Solid State Communications, 2007, 144, pp.94-97. 10.1016/j.ssc.2007.08.022 . hal-00212103

HAL Id: hal-00212103

<https://hal.science/hal-00212103>

Submitted on 2 Mar 2020

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Antiferromagnetism at V/Co(001) interfaces

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Abstract

Recent studies of x-ray magnetic circular dichroism (XMCD) at V/Co interfaces have determined the magnetic moments on V and Co atoms. The purpose of the present communication is to explain the strong induced polarization on V atoms in thin V layers deposited on Cu substrate and covered by Co atoms. Ab initio calculations performed with abrupt interfaces between Co and V do not lead to agreement with the XMCD results. Interfacial alloying between Co and V atoms increases greatly the moments on the interfacial V atoms and thus improves somewhat the agreement with the XMCD results.

PACS: 73.20.-r; 75.10.Lp; 75.70.Cn

Keywords: A. Magnetic films and multilayers; A. Surface and interfaces; A. Metals; A. Nanostructures

Recent ab initio calculations by Carrillo-Cázares et al. [1] and Hong [2,3] have obtained, for V submonolayer coverage on Co(001), a sizable magnetic moment on V atoms with an antiferromagnetic coupling between the V and Co atoms. Those ab initio calculations are in good semi-quantitative agreement with XMCD results of Huttel et al. [4].

Besides this, Carrillo-Cázares et al. [5] as well as Hong [2] performed calculations for a $V_{0.5}Co_{0.5}$ ordered alloy on Co(001) as well as one to three complete V monolayers on Co(001). As can be seen from the inspection of Carrillo-Cázares et al. [1,5] and Hong [2], for ordered $V_{0.5}Co_{0.5}$ alloy one monolayer thick on Co(001), similar results concerning the magnetic moments on V and Co atoms were obtained. However, for a complete V monolayer on Co(001) a major discrepancy arises, i.e. Hong [2] obtained a small magnetic moment for V atoms, a small decrease of the Co moment at the V/Co interface as well as an antiferromagnetic coupling between the V and Co atoms, whereas Carrillo-Cázares et al. [5] obtained a much greater moment for the V atoms with a ferromagnetic coupling between the V and Co atoms. The

discrepancy seems to arise from the relaxation effect taken into account by Hong [2]. In their paper, Carrillo-Cázares et al. [5] have used the same lattice parameters for Co and V: this is not correct.

In the present communication we perform fully relaxed calculations for V and Co atoms on Cu substrates. In order to perform the calculations we follow the growth procedure of Huttel et al. [4], i.e. the Co and V atoms are deposited on Cu(001) substrates. Following that we include in the calculations either the Cu substrate, for V at the interface with Cu, or *only* the experimental lattice parameter for Cu [6] in the “ $x-y$ ” plane, when the V atoms are separated from the Cu substrate by the Co film. The z direction is allowed to relax until the forces on the atoms become null. When the V monolayer is deposited on Co(001) it takes on, in the plane parallel to Co(001), the a_{Cu} lattice parameter; the lattice parameter perpendicular to Co(001) is obtained via force minimization. The magnetic moment on a second V layer decreases dramatically as compared to that for V/Co(001). Then we considered an ordered $V_{0.5}Co_{0.5}$ alloy one layer thick on Co(001). Once this had been done we considered the system Co/V/Cu(001) following the geometry used by Huttel et al. [4]. However the results obtained in this case do not agree with the

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Table 1

Magnetic moments (in μ_B) and z atomic positions (in a.u.) with respect to the Co_1 layer at the center of the Co slab of seven layers (denoted as 0.00), for V_n layers ($n = 1, 2$) on $\text{Co}(001)$; (a) one V monolayer on fcc $\text{Co}(001)$ and (b) two V layers on fcc $\text{Co}(001)$

	(a) V/Co(001)		(b) 2V/Co(001)	
	μ	z	μ	z
V2			-0.03	16.985
V1	-0.26	13.071	-0.20	13.162
Co4	1.34	9.670	1.35	9.606
Co3	1.78	6.521	1.75	6.481
Co2	1.77	3.229	1.76	3.214
Co1	1.77	0.000	1.76	0.000

Table 2

Magnetic moments (in μ_B) and z atomic positions (in a.u.) with respect to the Co_1 layer at the center of the Co slab with seven layers (denoted as 0.00), for an ordered $\text{V}_{0.5}\text{Co}_{0.5}$ alloy one monolayer thick on $\text{Co}(001)$

	z	μ_B
V	12.958	-1.82
Co	12.833	1.29
Co4a	9.779	1.34
Co4b	9.779	1.34
Co3a	6.467	1.70
Co3b	6.500	1.79
Co2a	3.244	1.72
Co2b	3.244	1.70
Co1a	0.000	1.70
Co1b	0.000	1.76

In this calculation two inequivalent atoms per layer have been considered.

experimental results because the polarizations obtained for the V atoms are rather low as compared to the $1.2\mu_B$ value obtained by Huttel et al. [4]. In view of the fact that an ordered $\text{V}_{0.5}\text{Co}_{0.5}$ alloy one layer thick displays a sizable magnetic polarization on V atoms, we finally considered a configuration with this ordered alloy at the interface between V and Co.

We have used a pseudopotential plane wave package [7] to perform the calculations. This program is based on density functional theory (DFT). The calculations are performed with the Perdew–Burke–Ernzerhof [8] exchange–correlation functional. The Monkhorst–Pack scheme was used to define the k points and calculations for each slab are performed with a grid of $8 \times 8 \times 1$ mesh in k space. The energy cut-off 35 Ryd was used for the plane wave expansion of the pseudowavefunctions (480 Ryd for the charge density and potential).

Calculations were performed in the slab geometry approach with two types of configurations: either a slab of seven layers of Co atoms (with the lattice parameter of Cu in the x - y plane) sandwiched by one or two V layers or a surface ordered $\text{V}_{0.5}\text{Co}_{0.5}$ alloy one monolayer thick; or a slab of seven layers of Cu atoms in contact with V atoms and sandwiched by Co atoms. More precisely we have performed calculations for the following systems: (1) $V_n/\text{Co}_7/V_n$, $n = 1, 2$; (2) $\text{V}_{0.5}\text{Co}_{0.5}/\text{Co}_7/\text{V}_{0.5}\text{Co}_{0.5}$; (3) $V_n/\text{Cu}_7/V_n$, $n = 1, 2$, $\text{Co}_n/\text{V}_2/\text{Cu}_7/\text{V}_2/\text{Co}_n$, $n = 1, 2$; and finally (4) $\text{Co}_n/\text{V}_{0.5}\text{Co}_{0.5}/\text{V}/\text{Cu}_7/\text{V}/\text{V}_{0.5}\text{Co}_{0.5}/\text{Co}_n$, $n = 1, 3$.

Table 3

Magnetic moments (in μ_B) and z atomic positions (in a.u.) with respect to the Cu_1 layer at the center of the slab (denoted as 0.00) for: (a) the fcc $\text{Cu}(001)$ surface; (b) one V monolayer on fcc $\text{Cu}(001)$ substrate; (c) two V layers on fcc $\text{Cu}(001)$ substrate; (d) one Co monolayer on $\text{V}_2/\text{Cu}(001)$; and (e) two Co layers on $\text{V}_2/\text{Cu}(001)$

	(a) Cu(001)	(b) V	(c) 2V	(d) Co/2V		(e) 2Co/2V	
	z	z	z	μ	z	μ	z
Co2						1.91	25.013
Co1				1.33	21.734	1.49	22.002
V2			18.294	-0.31	18.418	-0.19	18.393
V1		14.385	14.487	-0.03	14.506	-0.07	14.481
Cu4	10.545	10.664	10.672	0.00	10.660	-0.00	10.643
Cu3	7.089	7.096	7.099	0.00	7.087	0.00	7.079
Cu2	3.536	3.555	3.550	0.00	3.543	0.00	3.539
Cu1	0.000	0.000	0.000	0.00	0.000	0.00	0.000

The experimental lattice parameter of bulk Cu, equal to 6.81 a.u. [6], is used in the “ x - y ” plane. First we calculate the electronic structure of a film of nine (eleven) layers made of seven layers of Co sandwiched by one (two) layers of V. We have therefore the following geometry: $V_n/\text{Co}_7/V_n$, for $n = 1, 2$. In Table 1 we report the values obtained after relaxations, the z values (in a.u.) being the distances from the central Co layer (Co_1) (denoted as 0.00). We report both the z components (in a.u.) of these Co and V layers and their corresponding magnetic moments. In agreement with Hong [2] we obtain an antiferromagnetic coupling at the V/Co interface. However the magnetic moment is larger in the present calculation ($0.26\mu_B$) as compared to Hong’s result ($0.05\mu_B$). Thus it can be said that the magnetization on the V atoms is definitely very sensitive to the distance from its magnetic neighboring atoms. For two layers of V atoms at the top of the Co film there is a clear decrease of the induced polarization (Table 1). The surface V layer remains only marginally polarized.

In a second calculation we considered a film of nine layers made of seven layers of Co atoms sandwiched with an ordered $\text{V}_{0.5}\text{Co}_{0.5}$ alloy, one layer thick. For this configuration $\text{V}_{0.5}\text{Co}_{0.5}/\text{Co}_7/\text{V}_{0.5}\text{Co}_{0.5}$, it is clear that we have to consider calculations with two inequivalent atoms per layer. The results obtained are displayed in Table 2. Contrary to the case for the previous system with one V monolayer on $\text{Co}(001)$ for which the induced magnetic polarization on V atoms was marginal, in the present case the induced polarization is as high as $1.82\mu_B$. It is also seen that the V atoms do not stay in the same surface plane as the Co atoms: they are pushed outwards a little bit. This outwards relaxation is similar to the one reported by Hong [2].

Then we tried to recover the magnetic moments reported in the last line of Table 1 of Huttel et al. [4]. It is difficult to compute for the configuration 7 ML Co/1.8 ML V/Cu. Thus we have replaced it by the following geometrical configuration: n ML Co/VV/Cu with $n = 1, 2$. Before doing this calculation we first performed calculations for the Cu slab, V/Cu(001) and VV/Cu(001). The results are reported in Table 3. It can be seen that for these three configurations no magnetic moments were depicted. Afterwards, we considered one and two Co layers on

Table 4

Magnetic moments (in μ_B) and z atomic positions (in $a.u.$) with respect to the center of the slab (denoted as 0.00), for (a) Co/CoV/V/Cu(001), (b) 2Co/CoV/V/Cu(001) and (c) 3Co/CoV/V/Cu(001)

Co/VCo/V			2Co/CoV/V			3Co/CoV/V			4Co/CoV/V		
μ		z	μ		z	μ		z	μ		z
Co5a									1.91		31.193
Co5b									1.91		31.180
Co4a						1.92	27.887		1.72		28.094
Co4b						1.92	27.887		1.72		28.094
Co3a			2.01	24.729		1.81	24.823		1.82		24.805
Co3b			1.84	24.678		1.67	24.790		1.68		24.772
Co2a	1.17	21.447	1.27	21.600		1.16	21.466		1.17		21.544
Co2b	1.17	21.447	1.27	21.600		1.16	21.466		1.17		21.544
Co1	0.55	18.529	0.26	18.302		0.40	18.218		0.25		18.452
V2	-0.85	18.374	-0.63	18.417		-0.74	18.416		-0.69		18.302
V1b	0.10	14.589	0.05	14.527		0.02	14.506		0.01		14.541
V1a	0.10	14.589	0.05	14.527		0.02	14.506		0.01		14.541
Cu4a	0.01	10.768	0.00	10.722		0.00	10.699		0.00		10.732
Cu4b	0.00	10.772	0.00	10.713		0.00	10.688		0.00		10.723
Cu3a	0.00	7.157	0.00	7.132		0.00	7.124		0.00		7.123
Cu3b	0.00	7.157	0.00	7.132		0.00	7.124		0.00		7.123
Cu2a	0.00	3.575	0.00	3.565		0.00	3.565		0.00		3.559
Cu2b	0.00	3.575	0.00	3.565		0.00	3.565		0.00		3.559
Cu1a	0.00	0.000	0.00	0.000		0.00	0.000		0.00		0.000
Cu1b	0.00	0.000	0.00	0.000		0.00	0.000		0.00		0.000

VV/Cu(001). Again the two chemical configurations were fully relaxed by minimization of the forces.

A small induced polarization on V atoms at the Co-V interface, nearly equivalent to that obtained in Table 1, was obtained, i.e. $0.31\mu_B$ for one Co overlayer and $0.19\mu_B$ for two Co overlayers. The magnetic moment on the V monolayer at the interface with Cu remains rather small. Like in Table 1 the magnetic couplings between Co and V atoms are of antiferromagnetic type. However this induced polarization is totally at odds with those reported by Huttel et al. [4] but in full agreement with the previously reported induced polarization on V monolayers and bilayers of V on Co(001). Therefore we strongly believe that the present calculation gives the correct values of the induced polarization. From that, it can be said that a model with an abrupt interface between Co and V is not suitable for explaining the XMCD results. Let us remember that it was pointed out in Table 2 that a large induced magnetic moment was obtained on V atoms for an ordered $V_{0.5}Co_{0.5}$ alloy one monolayer thick on Co(001) substrate. Thus we believe that such a chemical configuration may improve the agreement with the XMCD results.

In order to check this point we go back to the results obtained by Carrillo-Cázares et al. [5] and Hong [2] concerning the $V_{0.5}Co_{0.5}$ ordered alloy on Co(001). In that case the induced polarizations on V atoms are respectively $1.67\mu_B$ [5] and $1.19\mu_B$ [2] for an ordered $V_{0.5}Co_{0.5}$ alloy one monolayer thick. Results reported in Table 2 confirm this tendency. Following this clue we performed calculations with the following geometrical configurations: n ML Co/ $V_{0.5}Co_{0.5}$ /V/Cu(001) with $n = 1, 2, 3, 4$. Again, here, we have performed calculations with two inequivalent atoms per layer. The results reported in Table 4 present some interesting features, particularly as regards the induced polarization on the V atoms.

The induced V polarization can be as high as $0.85\mu_B$ with an antiferromagnetic coupling with the Co atoms. This value has to be compared with the value $1.2\mu_B$ reported in the last line of Table 1 of Huttel et al. [4].

We have also considered the case with two layers of CoV ordered alloy, i.e. Co/2($V_{0.5}Co_{0.5}$)/V/Cu7/V/2($V_{0.5}Co_{0.5}$)/Co. This configuration is marginally less stable (0.3 mRyd/atom) than the non-alloyed configuration Co₂/V₂/Cu₇/V₂/Co₂, so it can clearly exist at the temperature at which the XMCD experiment was performed. However, although the polarization on V atoms remains high, this new configuration is clearly at odds with XMCD results, because the magnetic moments on the Co atoms are now clearly killed. Also we have examined a possible onset of magnetism in rather dilute V atoms on Cu substrate following XMCD results of Huttel et al. [9]. Indeed, for V impurity in Cu we have obtained a sizable magnetic moment. However, magnetization is killed when the V concentration increases, so this type of alloying does not provide any suitable answer.

To summarize, it can be said that in the present paper we have tried to recover the experimental values obtained by Huttel et al. for the magnetic moments on Co and V of 7 ML Co/1.8 ML V/Cu. Sizable magnetic polarization on V atoms can be obtained only if we consider Co-V alloying at the Co/V interface.

Acknowledgements

We thank B. R. Malonda-Boungou for fruitful discussions and advice. Part of this work was performed when S. Meza-Aguilar was on leave at The Abdus Salam International Center for Theoretical Physics.

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