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Spin polarization of Cr monolayers on W(10 k) vicinal surfaces

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Abstract

The magnetism of Cr/W stepped surfaces is investigated using the self-consistent tight-binding method in the unrestricted Hartree–Fock approximation with a Hubbard Hamiltonian. These structures exhibit local magnetic moments with the lowest values on the kink atoms and the highest on the edge atoms, owing to the coordination. The local moments of the kink atoms are frustrated due to the ferromagnetic coupling with their nearest neighbours. The net magnetization increases as a function of the step length.

1. Introduction

During the last few years, considerable effort has been devoted to understanding the interplay between structure and magnetism in thin-film systems since they are by no means independent. This is evident in transition metals such as Cr, which exhibits an antiferromagnetic (AF) behaviour in its bulk form with a magnetic moment $0.59 \mu_B$, whereas its surface has a ferromagnetic (F) structure with a local magnetic moment of about five times the bulk value [1–4]. Experimentally Klebanoff *et al* [5] obtained a closer value of about $2.4 \mu_B$. Recently, Nakajima *et al* [6] confirmed the possibility of a ferromagnetic state of a Cr(001) surface. They observed two peaks below the Fermi level in the normal-emission photoelectron spectra, in agreement with the observation of Klebanoff *et al* [5]. They related the periodicity of the energy-band dispersion along the [001] direction to the AF structure of Cr. Intensive studies have been carried out using different experimental techniques for Cr monolayers (MLs) on Fe(001) substrates due to their technological applications [7–9]. However, there is a considerable disagreement among the experimental results. This is related to the fact that magnetism is highly sensitive to the interface corrugations that depend on the experimental preparation conditions [10].

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The effect of interface defects on the spin density wave (SDW) in Cr has been discussed by a number of authors [11–16]. Several efforts were devoted to studying the magnetism of Fe(Cr) on Cr(Fe) vicinal surfaces [17–19]. The net magnetization of this structure decreases as the step length increases. Recently, the magnetic structure has been studied for Cr ML on vicinal V surface, which is stepped relative to the (001) orientation by a monolayer [20]. Unlike the case of Cr MLs on Fe vicinal surfaces, the net magnetization in Cr/V stepped structure increases as the step length increases. This could be ascribed to the difference in the nature of the ground state of Fe and V.

The geometrical structure of the substrate also affects the magnetic structure of the adsorbed Cr layers. A study by Blügel [21] has shown that Cr MLs adsorbed on Pd(001) substrates exhibit a $c(2 \times 2)$ AF magnetic configuration. This structure was also obtained by the calculation of angle-resolved photoemission spectra using FLAPW. The shift of the layer-by-layer-like contributions to the photocurrent were used to estimate the hybridization with the Pd host [22]. Though the net magnetization on the surface is zero at Cr/Pd(001) systems, a nonzero residual magnetization has been obtained for Cr overlayers adsorbed on Pd vicinal surfaces due to their ferrimagnetic configuration [23].

In the present study, we consider the W 5d transition metal as a substrate. Tungsten is known to be a paramagnet in its ground state. However, several experimental studies revealed the possibility of magnetizing such materials when they are brought in contact with ferromagnetic materials [24–26]. The structural and magnetic properties of the Fe/W(011) system were studied using the FLAPW method [27, 28]. The magnetic moments of the Fe surface layer were found to be close to that of the bulk value in the case of a ML system, while it considerably increases in bilayer and trilayer systems. Experimental investigations have shown that a short-range ferromagnetic order ~ 4 Å exists above T_C in the 1.5 ML Fe films adsorbed on W(001) substrates [29]. Recently, a profound study using the FLAPW method has revealed different characteristics between ultrathin Fe/W(110) and Fe/W(001) magnetic films [30]. The origin of this difference could be related to the symmetry and crystal-field effect that played a crucial role in the Fe–Fe and Fe–W interlayer interactions. In a previous study, we investigated the magnetic structure of Fe MLs on vicinal W substrates that was found to be highly affected by the corrugation of the surface [31].

In this study, we are concerned with Cr/W(10 k) stepped systems. The growth of Cr on W(110) and W(100) was studied by Berlowitz and Shinn from the ML range to a couple of MLs [32, 33]. The adsorption experiments showed that the bonding of Cr on W in both orientations is stronger than Cr itself.

2. Calculation method

The magnetic structures of the present systems are calculated using a self-consistent real space tight-binding method in the Hartree–Fock approximation of the Hubbard Hamiltonian. Our calculations in this method are based on the local density of states (LDOS) of the d band. Using the recursion method [34] we can determine $n_i(\varepsilon)$, which is the LDOS of the i th site. The spin polarized local density of states (SPLDOS) with spin σ of the i th site, $n_{i\sigma}(\varepsilon)$, is determined by using the Hubbard Hamiltonian for d electrons, which proved to be successful for most transition elements, where its diagonal terms are given by [35]:

$$\varepsilon_{i\sigma} = \varepsilon_d^0 + U\Delta N(i) - \frac{1}{2}\sigma J\mu(i) \quad (1)$$

for the atomic site i with spin σ and intrasite exchange and direct Coulomb integrals J and U , respectively. The number of d electrons $N(i)$ and the local magnetic moment $\mu(i)$ at the site

Table 1. The magnetic moments, in units of μ_B , for a Cr surface atom and W atoms at the sublayers, W(S - 1) and W(S - 2), in the (001) and (011) orientations.

	$\mu(S)$	$\mu(S - 1)$	$\mu(S - 2)$
(001)	3.39	-0.87	0.31
(011)	+3.57	+0.44	+0.13
	-3.57	-0.44	-0.13

i are given by

$$N(i) = \langle n_{i\uparrow} \rangle + \langle n_{i\downarrow} \rangle \quad (2)$$

$$\mu(i) = \langle n_{i\uparrow} \rangle - \langle n_{i\downarrow} \rangle \quad (3)$$

which are determined using the spin polarized density of states $n_{i\sigma}(\varepsilon)$. It is calculated with the recursion method [34], by requiring

$$\langle n_{i\sigma} \rangle = \int_{-\infty}^{\varepsilon_F} n_{i\sigma}(\varepsilon) d\varepsilon. \quad (4)$$

The charge transfer between different sites is given by

$$\Delta N(i) = N(i) - N_d \quad (5)$$

where N_d is the average number of d electrons at each site. If we impose local charge neutrality ($\Delta N(i) = 0$) by considering shifts Ω_i in the diagonal terms $\varepsilon_{i\sigma}$, then the term $U_i \Delta N(i)$ in equation (1) is replaced by Ω_i . This type of approximation has been successfully applied by Victora and co-workers [36, 37]. We use the canonical tight-binding parameters that result from the atomic sphere approximation of Andersen [38]. In this model the hopping parameters are spin-independent and restricted to d-type electrons. They are given explicitly [39] as the inverse fifth power of the interatomic distance R_j between j th neighbouring atoms:

$$dd(\sigma, \pi, \delta)_j = (6, -4, 1) \times (dd\delta)_1 (R_1/R_j)^5 \quad (6)$$

and they are chosen in order to recover the d bandwidth of Varma and Wilson [40]. Equations (1) and (3) are solved self-consistently and the procedure is stopped when the $\mu(\text{output}) - \mu(\text{input})$ is less than 10^{-4} .

3. Results and discussion

In this section we present the results of the magnetism of Cr MLs adsorbed on W semi-infinite vicinal surfaces of (10k) orientations, where $k = 1, 3, 5, 7, 9, 11$ and 13 . These surfaces are stepped relative to the (001) orientation by a ML forming a terraced shaped structures. Both Cr and W have BCC structures with lattice constants 5.41 and 5.98 au, respectively, and they have five d electrons [41]. The exchange integral of Cr, J_{Cr} , is adjusted to recover its bulk magnetic moment of $0.59 \mu_B$. However, that of W is obtained from LMTO calculations by Christensen [42] since it has a paramagnetic ground state.

First, for purposes of comparison, we start to investigate the magnetism of the Cr/W(001) system. In this orientation, all the sites are equivalent in each layer. Thus we considered one atom per layer to calculate the local magnetic moments. Table 1 displays the local magnetic moments at the surface, $\mu(S)$, the interfacial layer, $\mu(S - 1)$, and the subinterfacial layer, $\mu(S - 2)$. The surface magnetic moment, $3.39 \mu_B$, is considerably enhanced from that at the pure Cr surface, which is found to be about $2.79 \mu_B$ [43]. This is attributed to the increase in the interatomic distance in the Cr layer to meet that of the substrate. As a result of the hybridization between the d bands of Cr atoms with those of W at the interfacial layer, the

latter exhibits an appreciable induced magnetic moment, about $-0.87 \mu_B$. The system is found to exhibit an interlayer AF coupling owing to the AF ground state of bulk Cr.

The (101) orientation is considered as a facet of the (001) orientation. We considered two atoms per layer in our calculations of the local magnetic moment at this orientation, one at the corner and another at the centre. Table 1 displays the local magnetic moments of the Cr surface layer and the other two W sublayers below. The surface local magnetic moments are 3.57 and $-3.57 \mu_B$, which are larger than the surface magnetic moment at the (001) orientation. This is ascribed to the kind of neighbours in each case. At the (101) orientation, there are six first nearest neighbours for the surface atom, four Cr and two W atoms. However, in the case of the (001) orientation, the Cr surface atom has four first nearest neighbours of W, whereas the second nearest neighbours are Cr atoms. Since the Cr–W distance in the (001) orientation is smaller than the Cr–Cr distance, the Cr–W d-band hybridization is more pronounced than that of Cr–Cr, which explains the smaller value of the magnetic moment at this orientation. While the (001) surface layer exhibits a ferromagnetic structure, the (101) surface exhibits a $c(2 \times 2)$ AF structure, which corresponds to a zero net magnetization. Regarding the induced local magnetic moments of W atoms, they are smaller in the (101) orientation since most of their first nearest neighbours are W atoms, which makes the effect of W–Cr d-band hybridization less effective in this orientation. However, unlike the case of the (001) orientation, the interlayer coupling is found to be ferromagnetic in the (101) orientation.

The high-index orientations are vicinal surfaces of terraced shapes. The width of the planes depends on the experimental preparation [44]. The corrugation of a surface is believed to strongly affect the magnetic mapping of the system. Random terraces are likely to occur to minimize the surface free energy by maximizing the surface configuration entropy. However, the terraces considered in this context with regular orientations can be prepared by cutting or polishing the (001) low-index plane. Here we present a study of the magnetism of the $(10k)$ high-index orientations with $k = 3, 5, 7, 9, 11$ and 13. The (103) orientation is a vicinal surface of two inequivalent sites, one at the edge and another at the kink of the step (figure 1(a), two cells). Therefore, the local magnetic moment at the edge is found to be larger since its coordination number is less than that of the kink atom, four first nearest neighbours for the former and six for the latter. Although the two atoms are in second-nearest-neighbouring positions with respect to each other, they are antiferromagnetically coupled, which is defined as a frustration of the coupling. The coupling is also frustrated between the magnetic moment of the kink atom with one of the W atoms below that sits in a first-nearest-neighbouring position. This frustration is ascribed to the fact that the kink atom sits in a first-nearest-neighbouring position with the edge atom in the adjacent step, see figure 1(a). This behaviour is the same as that of Cr/V stepped structures [20]. This can be attributed to the fact that the substrates of W and V are paramagnetic materials that exhibit induced AF behaviour in the proximity of Cr. In the case of the (105) orientation, there are three inequivalent atoms per step. The behaviour of the edge and the kink atoms are the same as in the case of (103) orientation. However, in the (105) orientation, there is an interior atom that couples ferromagnetically with the edge atom and antiferromagnetically with the kink atom. The interior atom has four W first nearest neighbours, which means a stronger Cr–W d-band hybridization than in the case of the edge atom, which has also four nearest neighbours, but two of them are W atoms and the other two are Cr. This explains the smaller value of the magnetic moment for the interior atom as compared to the edge atom. However, the reason for the larger magnetic moment of the kink atom as compared to that of the interior atom, in spite of its larger coordination, is due to the induced moment acquired from the edge atom in the proximity. As the step length increases, the number of atoms that have ferromagnetically coupled moments increases and consequently the effect of the kink atom decreases.

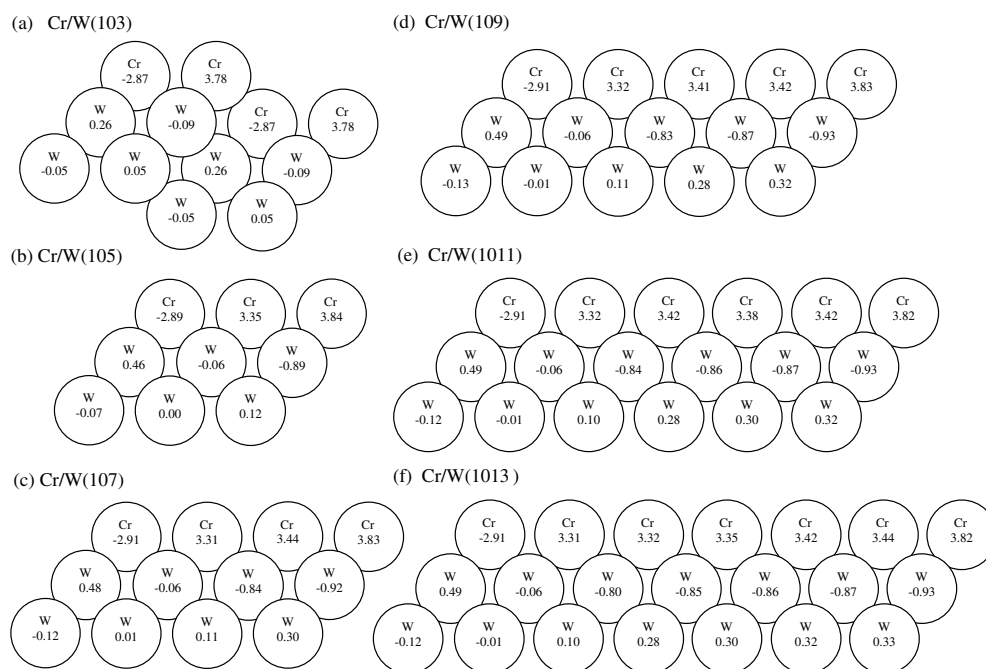


Figure 1. Local magnetic moments, in units of μ_B , for a Cr/W stepped structure at (103), (105) and (107) orientations. Only the surface Cr layer and two W sublayers of the substrate appear in the projection (100) plane. (a) Double-cell structure; (b) and (c) single-cell structures.

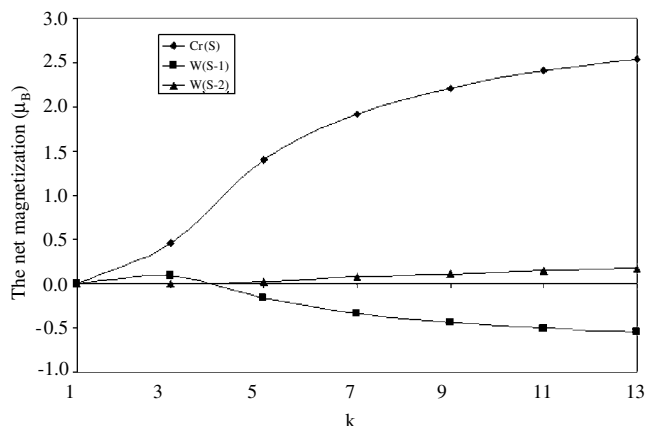


Figure 2. The net magnetization per atom (in units of μ_B) as a function of the step length, k , for a Cr overlayer, W interfacial layer and subinterfacial layer.

Figure 2 displays the net magnetization as a function of the step length for the overlayer, Cr(S), the interfacial layer, W(S-1), and the subinterfacial layer, W(S-2). The net magnetization increases as a function of the step length, where the values range from zero in the (101) orientation to $2.54 \mu_B$ in the case of the (1013) orientation. The net magnetization is expected to increase gradually as a function of k values. The inclination of the vicinal surfaces decreases as a function of k , i.e. 45° for $k = 1$ and 4.4° for $k = 13$. The value of the net

magnetization approaches that of the flat (001) surface asymptotically as k approaches infinity, which corresponds to zero inclination. This behaviour agrees with that of Cr/V and V/Mo systems [20, 45], whereas the case is the opposite in the Fe/W and Fe/Mo systems [31, 46]. This behaviour can be interpreted as follows: since Cr and expanded V [47] have AF ground states, the moment of the kink atom in a step is antiferromagnetically coupled with that of the edge atom in the adjacent step whereas it is ferromagnetically coupled with the moments of the other atoms. Therefore, as the step length increases, the number of atoms with moments pointing in the same direction increases and consequently the net magnetization increases. In addition, the net magnetization of W sublayers increases also as a function of k with an AF interlayer coupling, figure 2.

4. Conclusions

We investigated the magnetic structure of Cr/W stepped systems using the tight-binding method in the unrestricted Hartree–Fock approximation of the Hubbard Hamiltonian. In this study, we calculated the magnetic moment of a Cr/W(001) system first for the sake of comparison. The local magnetic moment of Cr is considerably enhanced by five times its bulk value and it is antiferromagnetically coupled with appreciable induced magnetic moments of W. In stepped surfaces the net magnetization per layer increases as a function of the step length, starting from zero at the (101) orientation and reaching $2.54 \mu_B$ for the (1013) orientation, which is expected to increase asymptotically towards the value of the (001) orientation as k approaches infinity.

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