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Magnetic structure of Cr/Ir vicinal systems

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Abstract

The magnetism of Cr/Ir vicinal systems is investigated using the self-consistent tight-binding method in the unrestricted Hartree–Fock approximation with the Hubbard Hamiltonian. These structures exhibit a ferromagnetic structure of unequal local magnetic moments with the lowest values on the kink atoms and the highest on the edge atoms. The net magnetization decreases as a function of the step length.

1. Introduction

Magnetism in transition-metal systems has become the interest of most theoretical and experimental investigations due to the sensitivity of this property to the structure and design of the system. There is a significant dependence between magnetism and structure in transition-metal systems. There are several factors that affect the magnetic structure of the transition-metal system. Among these are the dimensionality, the neighbourhood, the change in the interatomic distance and the roughness of the surfaces. Chromium is one evident example that exhibits the dependence. Bulk Cr exhibits an incommensurate spin density wave (I-SDW) structure of magnetic moments:

$$\mu = \mu_0 \sin(Q_{\pm}r) \quad (1)$$

with an μ_0 of about $0.5 \mu_B$ /atom at 4.2 K and commensurate wavevector given by:

$$Q_{\pm} = \frac{2\pi}{a_{Cr}}(1 - \delta)[001] \quad (2)$$

where δ is a measure of the deviation from the commensurability [1]. Its (001) and (111) surfaces have ferromagnetic (F) structures with much larger magnetic moments than the bulk value [2–7], whereas (011) surfaces exhibit a $c(2 \times 2)$ configuration [4, 8]. The effect of interface roughness on the SDW in Cr has been discussed by a number of authors [9–12]. The magnetic configuration of several vicinal surfaces has been investigated for several

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structures such as Fe–Cr and Cr–V vicinal systems that are stepped relative to the (001) orientation by a monolayer [13–16]. The net magnetization is found to decrease as the step length increases in Fe–Cr systems, whereas it decreases in the case of Cr–V stepped structures. This behaviour is related to the difference in the nature of the ground states of Fe and V. Investigations of magnetic polarization are mostly restricted to bcc-stepped surfaces [9–16] and the magnetism of vicinal fcc surfaces has scarcely been investigated. A study was carried out recently by Khalifeh and Demangeat for Cr monolayers (MLs) adsorbed on stepped Pd surfaces that have fcc structure [17]. In their study, they obtained ferrimagnetic configurations for the metastable state with sizeable magnetic moments on the Cr sites for all the considered stepped surfaces. Another theoretical study for an fcc structure of Fe monolayers on Ir stepped surfaces was recently published [18]. The structure of Ir surfaces has been investigated experimentally for (001) and (110) orientations by several experimental techniques such as scanning tunnelling microscopy (STM) supported by low energy electron diffraction (LEED) and Auger electron spectroscopy (AES). A study has been carried out for a Ir(001) surface and revealed a (1×5) structure using LEED analysis [19]. Other studies for Ir(110) surfaces have revealed the (1×3) construction [20] and stabilization via (331) facets [21, 22]. However, the present theoretical study is treating clean Ir surfaces with no technical defects. In the calculations we neglected any surface reconstruction of Ir substrates at which Cr atomic monolayers are expected to be epitaxially stabilized. This work aims to present a qualitative study of magnetism at such interfaces.

In this work we used the self-consistent tight-binding method in the Hartree–Fock approximation using the Hubbard Hamiltonian. The calculation method is presented in previous publications [23–28].

2. Results and discussion

In this section we present the results of the magnetic ordering of Cr monolayers adsorbed on Ir semi-infinite vicinal surfaces with orientations $(1\ 0\ 2n - 1)$, where $n = 1-5$. These surfaces are stepped from the (001) orientation by a monolayer forming terraced shaped structures. Chromium and Iridium have bcc and fcc structures with d-electrons 5 and 8, respectively [29]. The interatomic distances of bulk Cr and Ir are used to obtain the hopping integrals that recover the Varma and Wilson bandwidths [30]. Although bulk Cr has a bcc structure, the adsorbed atomic monolayer continues the fcc structure of the substrate. Thus the Cr hopping integrals are modified according to the new interatomic distances. The exchange parameter of Cr, $J_{\text{Cr}} = 0.591$ eV, is adjusted to recover its bulk magnetic moment at absolute zero temperature, $0.59 \mu_{\text{B}}$. However, the exchange parameter of Ir, $J_{\text{Ir}} = 0.52$ eV is taken from linear muffin-tin orbital (LMTO) calculations [31].

In this work, the local magnetic moment is calculated as the difference of the total number of spin up and spin down electrons. We neglect any relativistic effects since the spin–orbit contribution is very small in such systems. Bruno [32] has estimated the orbital contribution to the magnetization in transition-metal monolayers and it was negligible compared to the spin moments. A recent *ab initio* study of induced magnetism at 5d transition-metal W(011) surface has, therefore, also neglected this relativistic effect [33].

In this context, investigations were carried out first for the magnetism of the Cr monolayer on the Ir(001) surface. This system is found to exhibit a $c(2 \times 2)$ AF configuration in Cr overlayer as shown in figure 1. This figure represents a top view of a portion of the Cr/Ir(001) system. The magnetic moments of Cr atoms of the two inequivalent sites that are considered in the calculations are 3.5 and $-3.5 \mu_{\text{B}}$. This behaviour of in-plane AF coupling on the surface is ascribed to the AF ground state of bulk Cr since the Cr surface atoms are located in first

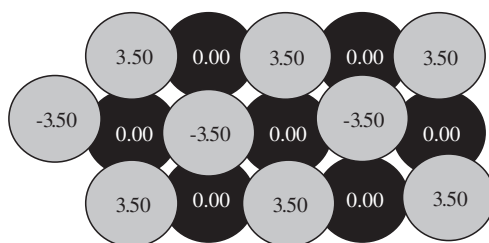


Figure 1. Top view of the (001) orientation, displaying the ferrimagnetic configuration at the surface. The local magnetic moments appear at Cr atoms (grey balls) in units of μ_B , whereas the atoms at the subsurface (black balls) introduce zero magnetism.

nearest neighbour positions due to the fcc structure of the substrate. As a consequence of the in-plane AF configuration, there are no induced magnetic moments acquired by Ir atoms at the interfacial layer. This is attributed to the zero net magnetization of the Cr surface layer. This behaviour agrees with the results of Cr/Pd(001) system, but with smaller surface local magnetic moments [34]. This could be related to the larger bandwidth of Ir, compared with Pd, which causes a lower magnetic moment for Cr atoms in the case of Ir substrates. This calculation, concerning 1 ML of Cr on Pd(001), has been extended to thicker Cr slabs by Khalifeh [34]. In his investigation two structures were obtained, a $c(2 \times 2)$ AF configuration and a $p(1 \times 1)$ F magnetic configuration, but the former was more stable. However, in our calculations, the $c(2 \times 2)$ AF configuration is the only solution obtained on the Cr monolayer adsorbed at Ir(001) surface. In the case of a Pd substrate, ferromagnetic solutions appeared on the Cr overlayer with less stability. This could be attributed to the large susceptibility of Pd and its tendency towards the ferromagnetic behaviour that enhances the appearance of the ferromagnetic solution in Cr/Pd overlayers.

Figure 2 displays the local density of states (LDOS) of the spin up and spin down electrons of the Cr surface atom in the Cr/Ir(001) system. This figure shows that the spin up electron occupation is larger than that of spin down, which is related to the magnetic behaviour of the surface. However, the LDOS of spin up and spin down electrons per Ir atom at the interfacial layer, figure 3, shows a mirror image symmetry that corresponds to a zero magnetic moment per atom. The above results are introduced to study the effect of roughness on these flat surfaces.

Here we introduce the roughness as a vicinal surface structure; the surfaces under consideration are of orientations $(1\ 0\ 2n - 1)$, where $n = 1-5$. These surfaces are stepped from the (001) orientation by monolayers of different step lengths, $k = 2n - 1$. Figure 4, in [18], displays the structure of these surfaces, which is given as an example that represents the (103) structure. Figures 4(a)–(e) represent the unit cells of (101), (103), (105), (107) and (109) vicinal structures in which the number of inequivalent sites are two, four, six, eight and ten, respectively. The calculations are carried out for the magnetic moments of the atoms at these inequivalent sites. The local magnetic moment is found to be the largest for the edge atoms that have the least number of nearest neighbours in such vicinal surfaces (see figures 4(a)–(e)). However, the kink atoms possess the lowest local magnetic moments since their coordination numbers are the largest relative to the other atoms in each unit cell. The interior atoms are found to possess local magnetic moments that lie between the moments of the edge and kink atoms. Thus, these vicinal systems exhibit ferromagnetic configurations, unlike the Cr/Ir(001) system that has a $c(2 \times 2)$ AF magnetic structure. Therefore, the (001) surface has a zero net magnetization whereas, at the vicinal surfaces,

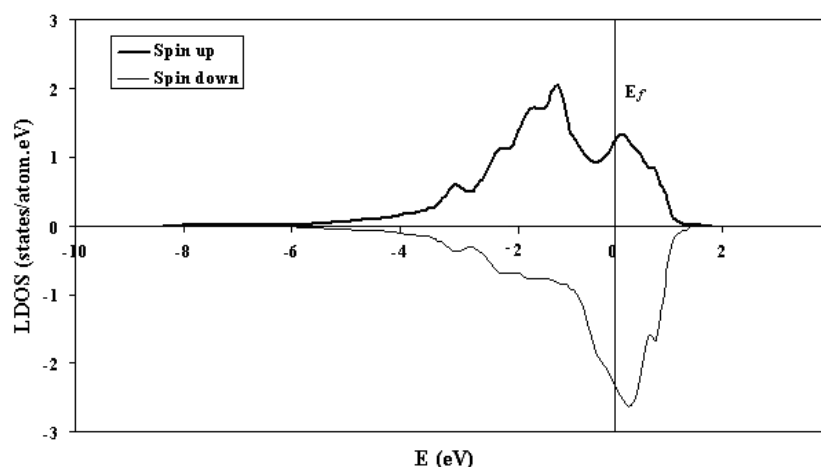


Figure 2. The local densities of states of spin up and spin down electrons for Cr surface atoms (S) in the (001) orientation.

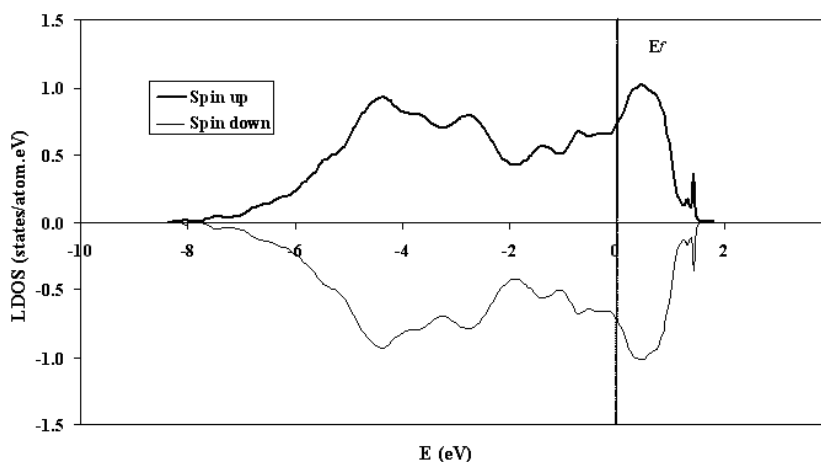


Figure 3. The local densities of states of spin up and spin down electrons for Ir interfacial layer atoms ($S - 1$) in the (001) orientation.

there is always a surface net magnetization due the unequal values of the magnetic moments. Superconducting quantum interference devices (SQUID) at very low temperatures should show this remaining magnetic moment on the surface. This has been already observed using SQUID and x-ray magnetic circular dichroism (XMCD) by Albrecht *et al* [35] in Cr/Ru(0001) superlattices. The surface net magnetization is found to decrease as a function of the step length as shown in figure 5. This behaviour agrees with that of the Cr/Pd vicinal system [17] since they both have fcc structures. However, this behaviour contrasts with that of the Cr/W vicinal system, which has a bcc structure, where the net magnetization increases as a function of the step length [36].

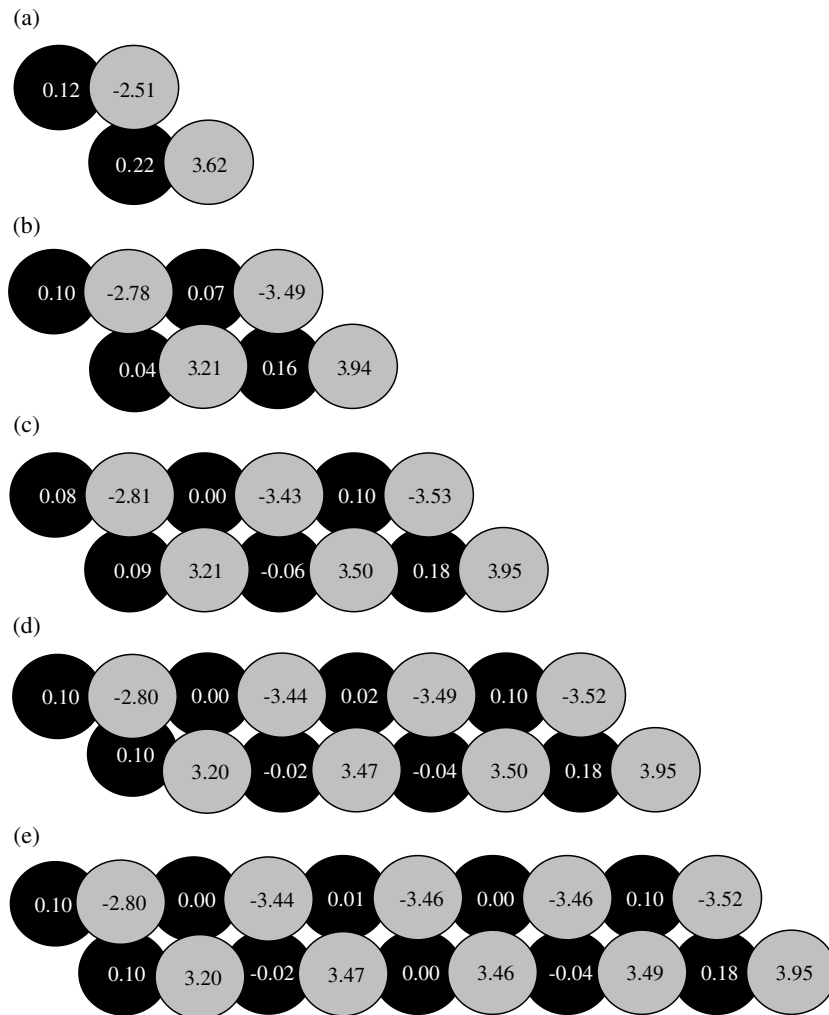


Figure 4. Top view of the surface layer (grey balls) and the interfacial layer (black balls) displaying the local magnetic moments, in units of μ_B , of the Cr surface atoms and the Ir interfacial layer for: (a) (101) orientation (two inequivalent sites per unit cell), (b) (103) orientation (four inequivalent sites per unit cell), (c) (105) orientation (six inequivalent sites per unit cell), (d) (107) orientation (eight inequivalent sites per unit cell) and (e) (109) orientation (ten inequivalent sites per unit cell).

3. Conclusion

The magnetic structure for Cr monolayers adsorbed at Ir(001) flat surfaces and Ir(1 0 2*n* - 1) vicinal surfaces with $n = 1-5$ has been investigated. The calculations were carried out using the tight-binding method within the Hartree–Fock approximation. In the study, we obtained an antiferromagnetic $c(2 \times 2)$ configuration at the Cr surfaces adsorbed on flat Ir(001) substrates with zero net magnetization at the Ir interfacial layer. However, Cr monolayers adsorbed at Ir vicinal surfaces exhibit a ferrimagnetic structure with an appreciable net magnetization for each system, that decreases as a function of the step length.

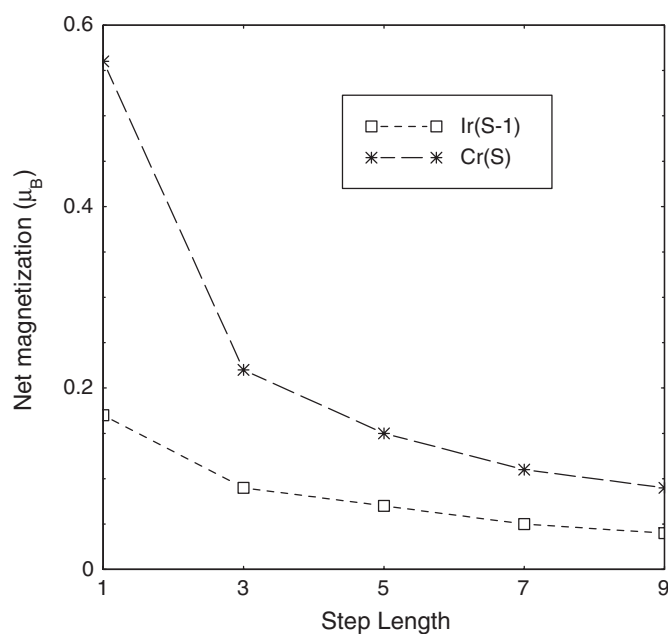


Figure 5. The net magnetization for the Cr(S) surface atoms and the Ir(S – 1) interfacial atoms as a function of step length.

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