

Magnetic properties of ultrathin films of Cr on W(001)

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1996 J. Phys.: Condens. Matter 8 4165

(<http://iopscience.iop.org/0953-8984/8/23/009>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.206

The article was downloaded on 13/05/2010 at 18:25

Please note that [terms and conditions apply](#).

Magnetic properties of ultrathin films of Cr on W(001)

A Boussendel and A Haroun

Institut de Physique, Université Ferhat Abbas, Sétif 19000, Algeria

Received 30 October 1995, in final form 12 February 1996

Abstract. We have investigated the magnetic properties of Cr layers adsorbed on W(001) by means of self-consistent tight-binding calculations in the framework of the Hubbard Hamiltonian within the unrestricted Hartree–Fock approximation. We have observed that the polarization appears at the Cr–W interface until the fourth plane is reached and the magnetic moment in the W interface decreases when the number of Cr layers increases. In all cases we obtain an antiferromagnetic coupling between Cr layers and Cr–W interfaces. The general results can be understood in terms of the competition between surface and interface effects.

1. Introduction

In recent years, an intense research effort has been made to achieve the realization and characterization of new materials obtained by deposition of a metal on a metal substrate. The magnetic properties have been especially thoroughly studied, due to the possible technological applications. Some of these artificially built systems seem to be simple and more predictable than others. Victora and Falicov [1] have discussed, in the framework of the tight-binding method, the pure semi-infinite Cr system and the case of one monolayer of Cr on Fe(001). In both cases, the semi-infinite system was modelled through a thick slab. An extension of up to five layers of Cr on Fe(001) was performed by Dorantès-Davila *et al* [2]. The Cr magnetic moment at the Cr/Fe(001) interface always preferentially aligns antiparallel to the nearest-neighbour (n.n.) Fe moment [3]. This type of polarization has also been obtained in the case of the moment at the Fe/W(001) interface [4]. Very recently Stoeffler and Gautier [5] determined the local magnetic moment distribution of thin films of Cr deposited on stepped Fe(001). Using the same type of Hamiltonian as used in this work, they found an antiferromagnetic coupling between the Cr and Fe atoms at the flat interface. The presence of a step induced frustration and complex magnetic arrangements [5, 6]. In this work we investigate the magnetic properties of Cr_n ($n = 1, 3$) layers on W(001). We use a self-consistent TB formulation of the Hubbard Hamiltonian in the unrestricted Hartree–Fock approximation taking into account only the d electrons. This approach is expected to provide valuable complementary information to the first main calculations of the magnetic properties of the system mentioned above.

2. Model and method of calculation

In this work, we used a tight-binding Hubbard Hamiltonian in the unrestricted Hartree–Fock approximation [7, 8]. The study of transition metals belonging to the middle of the

series and the main physical properties can be described by taking into account only the d electrons. The corresponding Hamiltonian is written as

$$H = \sum_{i,\sigma} E_{i\sigma} C_{i\sigma}^+ C_{i\sigma} + \sum_{i,j,\sigma} t_{i,j}^{\alpha\beta} C_{i\sigma}^+ C_{j\sigma} \quad (1)$$

where $C_{i\sigma}^+$ ($C_{j\sigma}$) refers to the creation (annihilation) operator for an electron with spin σ at atomic site i in the orbital α , and $t_{i,j}^{\alpha\beta}$ are the hopping integrals for d electrons hopping between sites i and j . The $t_{i,j}^{\alpha\beta}$ are the nearest-neighbour hopping integrals and have been fitted on the bulk pure element bandwidth [9]. We assume that the hopping integrals for hopping between two different types of atom are the geometric means of the pure element hopping integrals with the same interparticle distance [10]. We consider the interaction up to second neighbours. In the case of the Cr adsorbed on W(001), the lattice parameter presents an expansion of 9.6% compared to the bulk value. In this model, the hopping integrals are spin independent, whereas the spin-dependent diagonal terms are given by [7]

$$E_{i\sigma} = E_d^0 + U \Delta N_i - \sigma \frac{J}{2} \mu_i \quad (2)$$

where i is the index of the atomic plane and σ is the spin. E_d^0 is the d atomic level and can be chosen as zero. The exchange and effective direct intra-atomic Coulomb integrals, denoted by J and U respectively, are taken to be independent of the size of the slabs and of the position i ; U is taken from the work of Bandyopadhyay and Sharma [11], whereas the values of J have been fitted in order to recover the bulk magnetic experimental value ($0.59\mu_B$) [12]. Because bulk W is not magnetic, we have taken its J -value in accordance with Christensen *et al* [13]. N_d has been considered: $N_d(\text{Cr}) = 5$ and $N_d(\text{W}) = 5$ [14]. The local magnetic moment is given by

$$\mu_i = (N_i^+ - N_i^-) \mu_B \quad (3)$$

whereas the numbers of electrons $N_{i\sigma}$ are determined by

$$N_{i\sigma} = \int_{-\infty}^{E_F} n_{i\sigma}(E) dE. \quad (4)$$

The spin-polarized local density of states (SPLDOS) $n_{i\sigma}(E)$ is calculated by using the recursion method [15] with twelve levels of continued fraction. Previous studies [8, 16–18] have shown that this number of levels is a good compromise for reaching satisfactory convergence in reasonable computational time (which grows as the square of the number of levels). Note that we allow charge transfer ΔN_i between different atomic planes by requiring global charge neutrality:

$$\Delta N_i = \sum_{\sigma} (N_{i\sigma} - N_{i\sigma}^0) \quad (5)$$

where $N_{i\sigma}^0$ is the number of d electrons with spin σ of the bulk.

3. Results and discussion

3.1. The Cr/W system

In this section we report in table 1 the results obtained for the magnetic moment distribution of Cr_n ($n = 1, 3$) layers on a W substrate. The calculations have been done for along the (001) crystallographic face. The local magnetic moments and the electronic charges in each site have been calculated fully self-consistently.

Table 1. Magnetic moments (in units of μ_B) per atom of semi-infinite W(001) and Cr adsorbed layers: the labels $n\text{Cr}/\text{W}(001)$ refer to n -plane Cr films. The index I refers to the Cr–W interface.

	1Cr/W(001)	2Cr/W(001)	3Cr/W(001)
Bulk	0.00	0.00	0.00
W_{I-3}	0.10	0.08	0.08
W_{I-2}	-0.15	-0.13	-0.13
W_{I-1}	0.32	0.25	0.24
W_I	-0.85	-0.68	-0.66
Cr_I	3.35	2.78	2.70
Cr_{I+1}		-4.17	-3.53
Cr_{I+2}			4.30

Let us now comment on the results.

(1) The magnetic moments of the chromium surfaces increase, as a consequence of the band narrowing (associated with the reduction of the coordination number) for a partially filled d band.

(2) We obtain an antiferromagnetic (AF) coupling between Cr layers and the Cr–W interface (figure 1), and the same coupling between W layers (figure 1). In each Cr layer the atoms are coupled ferromagnetically. The same result was obtained in the case of Fe layers adsorbed on semi-infinite W(001) by Fabricius and Dreysse [4] using a tight-binding (TB) method.

(3) The local magnetic moment of Cr in all the observed layers is considerably larger than the bulk value.

(4) A reduction of the magnetic moment in the W interface is obtained when the number of chromium layers adsorbed on the W increases. This is reasonable because the surface of a semi-infinite W(001) system is paramagnetic.

4. Discussion

The general behaviour can be explained taking into account two factors. The first is a ‘surface’ effect due to the reduction of the coordination number for an atom at the surface. This induces a band narrowing leading to an increase of the magnetic moment, because in a tight-binding model the width w of the band is related to the square root of Z [19], where Z is the coordination number. The second factor is the interface effect. When a magnetic transition metal has an interface with a bulk non-magnetic material, the non-magnetic material becomes polarized near the interface and the magnetic material magnetic moment is diminished at the interface. This can be explained in terms of hybridization of the two metal orbitals. The reduction of magnetic moment of a Cr monolayer on a W substrate implies that the hybridization between Cr d and W d bands plays an important role in determining the Cr magnetism. The comparison with other calculations is complex. In the case of Cr/Fe interfaces, larger values of magnetic moments have been reported [5, 6]. This is not surprising: the W substrate is not polarized and the bandwidth is much larger than the bandwidths of ‘3d’ elements. These two effects act against magnetism.

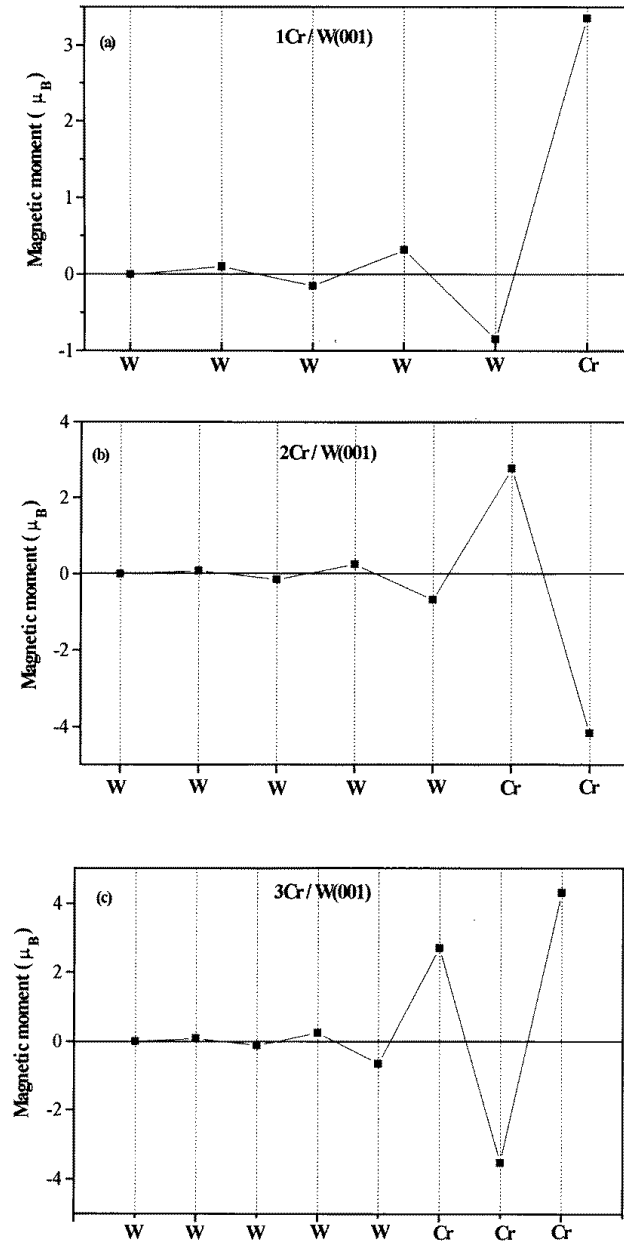


Figure 1. The magnetic moments of the atoms in the magnetic unit cell for: (a) 1Cr/W; (b) 2Cr/W; (c) 3Cr/W.

5. Conclusion

We have investigated the magnetic properties of Cr layers on a W substrate using a self-consistent tight-binding method. This study has shown the richness of the magnetic arrangements. The W atoms are shown to be polarized up to the fourth plane. The W

shows a very large polarization at the Cr–W interface. Moreover, for this case, in-plane AF solutions are present. The Cr polarization is AF with a rapid decrease when the number of chromium layers increases. In the absence of experimental results concerning the magnetism of Cr layers adsorbed on W(001), our results open up a new field for the magnetism of the Cr/W system.

Acknowledgments

We would like to thank the Laboratoire de Physique du Solide de l'Université de Nancy I for hospitality and Professor H Dreyssé for fruitful discussions at various stages of this work. We would like to thank also Drs J Dorantès-Davila, S Bouarab and S Ounnasser for helpful discussions.

References

- [1] Victora R H and Falicov C M 1985 *Phys. Rev. B* **31** 7335
- [2] Dorantès-Davila J, Mokrani A, Vega A, Rubio A, Demangeat C, Dreyssé H and Balbas L C 1991 *Surf. Sci.* **215/252** 51
- [3] Hillebrecht F U, Roths C, Jungblut R, Kisker E and Bringer A 1992 *Europhys. Lett.* **19** 711
- [4] Fabricius G and Dreyssé H 1996 to be published
- [5] Stoeffler D and Gautier F 1995 *J. Magn. Magn. Mater.* **147** 260
- [6] Vega A, Stoeffler D, Dreyssé H and Demangeat C 1995 *Europhys. Lett.* **31** 561
- [7] Pastor G M, Dorantès-Davila J and Bennemann K H 1988 *Physica B* **149** 22; 1989 *Phys. Rev. B* **40** 7642
- [8] Dreyssé H, Mokrani A, Bouarab S and Demangeat C 1991 *Surf. Sci.* **251/252** 41
- [9] Varma C M and Wilson A J 1980 *Phys. Rev. B* **22** 3795
- [10] Shiba S 1971 *Prog. Theor. Phys.* **46** 77
- [11] Bandyopadhyay T and Sharma D D 1989 *Phys. Rev. B* **39** 3517
- [12] Shirane G and Takei W J 1962 *J. Phys. Soc. Japan Suppl.* **B 3** 35
- [13] Christensen N E, Gunnarsson O, Jepsen O and Andersen O K 1981 *J. Physique Coll.* **49** C8 17
- [14] Papaconstantopoulos D 1986 *Handbook of the Band Structure of Elemental Solids* (New York: Plenum)
- [15] Haydock R 1980 *Solid State Physics* vol 35, ed H Ehrenreich, F Seitz and D Turnbull (New York: Academic) p 215
- [16] Gautier F and Stoeffler D 1991 *Surf. Sci.* **249** 265
- [17] Stoeffler D and Dreyssé H 1991 *Solid State Commun.* **79** 645
- [18] Bouarab S, Nait-Laziz H, Demangeat C, Mokrani A and Dreyssé H 1992 *J. Magn. Magn. Mater.* **102** L233
- [19] Mokrani A, Demangeat C and Dreyssé H 1990 *Phys. Rev. B* **42** 10