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Hubbard and Anderson periodic models for the description of imperfect low-dimensional FeCr magnetic systems

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Abstract

This paper presents the results of calculations of the magnetic moment distribution in the framework of the tight-binding Hubbard model and the Anderson periodic model for spatially nonhomogeneous systems (stepped surfaces of Fe and Cr, monolayer coverings on such surfaces). These data are used for a description of recent experiments with low-dimensional FeCr magnetic systems.

The substantial role of the effects of imperfections on the properties of low-dimensional magnetic systems underlines the importance of the development of the theory to describe such nonhomogeneous systems.

Ab initio calculations cannot properly describe the electronic structure of complex stratified systems, when the spatial homogeneity is broken in every plane. Therefore it is of considerable interest to use a model Hamiltonian approach, such as the Hubbard or the Anderson periodic model, to describe these systems.

The results obtained for the same systems within ab initio theory and the tight-binding model Hamiltonian approaches often appear to be in reasonable agreement. At the same time, with the model Hamiltonian method it is possible to describe much more complex objects that correspond to the properties of the systems under experimental investigation.

Each model Hamiltonian takes into account a specific set of interactions. It is of interest to compare the results obtained within the frameworks of different model Hamiltonians for the description of the same set of physical systems. This allows one to extract robust features of the electronic and magnetic structures, reproduced by different methods, and to separate them from features that are the consequence of the approximations used and the limitations of the relevant interactions accepted in different models.

Here we compare the results of calculations for spatially nonhomogeneous systems (stepped surfaces of Fe and Cr, monolayer coverings on such surfaces) in the framework of the tight-binding Hubbard model [1] and the Anderson periodic models [2]. The calculations were performed in the mean field approximation by real space methods.

At the vicinal ideal surfaces of Cr we obtain considerable enhancement of localized magnetic moments. This is connected with the diminishing numbers of nearest neighbors for surface atoms and the narrowing d-band width related to this. The surface magnetic moments are greater by about $0.5\mu_B$ within the Hubbard model than for the Anderson periodic model. However, for successive layers this difference does not exceed $0.05\mu_B$.

The enhancement of magnetic moments near the surfaces of Fe and Cr was recently confirmed by in-situ magnetometer measurements in the course of the growth of ultrathin Cr films on the Fe(001) surface [3]. For the adequate description of the electronic and magnetic structures of real systems investigated in this experiment, it was found to be necessary to take into account the roughness of the surface and the interface, and the lack of spatial homogeneity in the plane. This created interest in the calculation of stepped surfaces and surfaces with high Miller indices, since such systems can be considered as a first approximation to the real experimental structures.

Stepped Fe/Cr interfaces in 'wedge-shaped' configurations have also been investigated by different experimental groups in relation to the exchange magnetic coupling in Fe/Cr/Fe systems [4].

The distribution of magnetic moments for the stepped vicinal surfaces are shown in Fig. 1. Fig. 1(a) shows the results of calculations for the Hubbard model, and Fig. 1(b) those for the stepped surface within the Anderson periodic model. The two systems do not coincide; Fig. 1(a)

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shows the results of the magnetic moment calculations for surfaces with Miller indices (107). One can consider such surfaces as stepped where all the steps go down. In Fig. 1(b), due to periodic boundary conditions, the steps alternate up and down. However, there are some common features in these two cases.

(1) In each step the signs of the magnetic moments are opposite to those in adjacent steps. This can explain the small total magnetic moment of the Cr surface, as has been detected in spin-resolved photoemission experiments [5], and the nonzero splitting in experiments where local spin-split surface states have been determined [6]

(2) The magnitudes of the magnetic moments at the edges of each step turn out to be greater than those of the kink atoms. The number of nearest neighbors for the edge atoms is less than for the kink atoms, and this correlates with the enhancement of magnetic moments near the surface due to the decrease in the number of nearest neighbors for surface atoms.

(3) The magnetic moments of the surface atoms obtained within the Anderson periodic model prove to be less than within the Hubbard model. This difference is considerable for surface atoms and much less for successive atoms.

Monolayer coverings of stepped surfaces are of interest due to their applications for the protection of metal surfaces from gas absorption, which drastically changes their magnetic properties, and also because such systems allow one to simulate regularities that arise on the real rough interface of metals.

Fig. 2 shows the distribution of magnetic moments for a Cr monolayer on the stepped Fe (107) surface, obtained within the Hubbard model (a), and within the Anderson periodic model (b). It is worth noting that, as a rule, the Cr atoms of the monolayer and the Fe atoms of the substructure have opposite moments. The magnetic moments of the

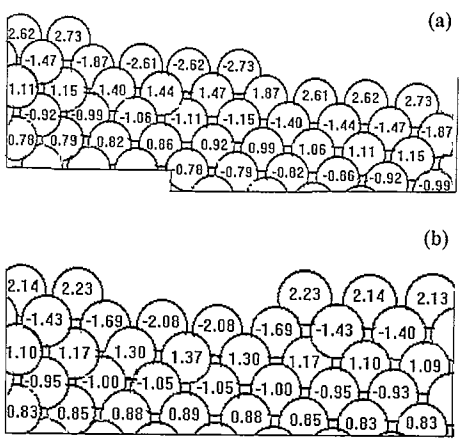

Fig. 1. Local magnetic moments (in units of μ_B) per atom for the vicinal stepped Cr surface (107) obtained within the framework of (a) the Hubbard model, and (b) the Anderson periodic model.

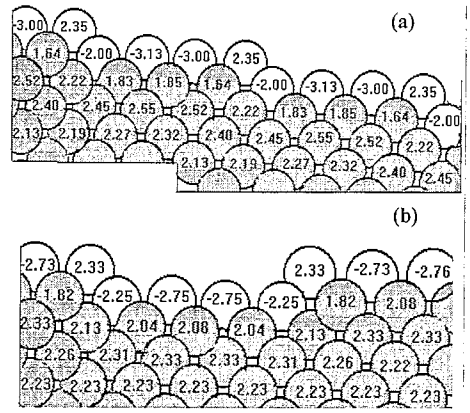

Fig. 2. Local magnetic moments (in units of μ_B) per atom for a Cr monolayer on the stepped Cr substrate obtained within the framework of (a) the Hubbard model, and (b) the Anderson periodic model.

Fe atoms at the interface prove to be less than those for the vicinal Fe surface. This causes a decrease in the total magnetic moment of the sample during Cr coverage in the experiments [3]. However, the value of the decrease can hardly be obtained without assumptions about the penetration of some Cr atoms through the Fe atoms to the depth of several lattice constants.

Note also that Cr atoms prefer antiferromagnetic ordering with respect to the nearest-neighbor Cr atoms. For stepped surfaces, a violation of ferromagnetic ordering in the Cr monolayer can occur due to frustration. For instance, the atoms at the step edges in Fig. 2(a) and (b) have moments opposite to those of other moments in the monolayer.

Table 1
Average local magnetic moment per atom in the layers for the Cr film with Fe atoms randomly filling half the sites on the perfect Cr(100) surface

Layer number	Magnetic moment (μ_B)	
	FM initial ordering	AFM initial ordering
1	−1.31	1.31
2	1.68	−1.73
3	−1.16	1.23
4	0.86	−1.01
5	−0.63	0.88
6	0.41	−0.81
7	−0.18	0.78
8	−0.05	−0.77
9	0.28	0.79
10	−0.51	−0.84
11	0.73	0.93
12	−0.98	−1.09
13	1.34	1.40
14	−2.09	−2.12

It is worth mentioning that the self-consistent solution for complex spatial nonhomogeneous systems often appears to be non-unique. For example, in Ref. [7], 16 different solutions for an Fe monolayer on the Cr (107) surface were obtained. These solutions have different energies. However, the difference between the energies for various configurations is quite small and some of the configurations can manifest themselves in the experiment as metastable. Thus, for the description of the ground state of such systems, all solutions should be carefully examined, and the energies compared.

It is also worth mentioning the average magnetic moments of successive layers when the Fe atoms fill randomly half the sites on the perfect 13-layer film of Cr(100). If we constrain the Fe polarization to be ferromagnetically (or antiferromagnetically) coupled with the free surface of the Cr film we obtain two solutions (Table 1) with a small difference in energy. Moreover, using a random modelling of the epitaxial process, a reasonable explanation of the experimental results of Turtur and Bayreuther [3] has been proposed [8].

In summary, we have calculated the local magnetic moment distribution for some spatially nonhomogeneous systems such as stepped Fe and Cr surfaces and monolayers on these surfaces within the framework of the Anderson periodic and Hubbard models. It has been shown that the main qualitative features of these distributions coincide. This gives support for the possibility of describing of real experiments with FeCr low-dimensional systems by these methods.

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