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Fe/Cr interface magnetism in the external magnetic field

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Abstract

A method of self-consistent calculation of magnetic ordering in low-dimensional metallic structures in the presence of an external magnetic field is developed on the basis of periodic Anderson model. Multitude of self-consistent solutions for the magnetic moments distribution in interface region leads to a hysteresis-like dependence of the average magnetic moment on value of the applied field. The shape of hysteresis loop calculated individually for Fe and for Cr atoms changes significantly depending on the structure of the interface region.

Keywords: Model Hamiltonian; Magnetic moments distribution; Hysteresis loop

New phenomena which were discovered in Fe/Cr multilayers have attracted a number of experimental methods for their investigations. However, the results and interpretation of these experiments, even obtained by similar methods, often contradict one to another [1]. One of the reasons of such contradictions is a sensitivity of the Fe/Cr multilayers properties to the interface morphology, which strongly depends on the details of preparation conditions. Theoretical calculations of the Fe/Cr interface structure, taking into account a roughness and interdiffusion, also demonstrated a very complex behaviour and existence of a number of self-consistent solutions with close energies [2,3]. That is why the problem of solution's stability relatively external perturbations, such as an external magnetic field, have a principal importance for these systems.

In this paper we report the results of magnetic structure calculations of Cr overlayer on a rough Fe surface within the collinear periodic Anderson model (PAM) in presence of the external magnetic field. The rough interface was constructed using 'epitaxy' algorithm [4,5], which fills sites of an ideal BCC lattice inside the prism $8 \times 8 \times 11$ by the Fe and Cr atoms using a special random procedure. Outside the prism we used periodic boundary conditions. The bottom layer (11) was uniform filled by the Fe atoms, and for modelling of a semi-infinite sample we accepted that the next layer (12) coincides with the previous. The algorithm parameters varying gives a possibility to create the surfaces and interfaces with a different but controlled roughness. For determination of average values the sample construction was repeated 20 times, so that every layer effectively contained $8 \times 8 \times 20 = 1280$ independent sites. Table 1 displays layer by layer the number of Fe atoms, Cr atoms, and empty sites for two Cr monolayers on the Fe substrate, which are obtained by 'epitaxy' algorithm with parameters, corresponding to the relatively smooth (SI) and rough (RI) interfaces. For each of these structures self-consistent calculations of the magnetic moments within PAM were performed. Due to s–d-interaction, which is taken into account in PAM, d-levels of the Fe and Cr atoms have a finite width Γ, which is a parameter of the model. Effectively, for every element (either Fe or Cr) we used three dimensionless parameters: $x = (E_0 - \varepsilon_F)/\Gamma$ determines the position of d-level relatively Fermi-level, U/Γ describes the Coulomb repulsion on the site in Hartree–Fock approximation, and V/Γ is the hoping integral. The parameters were chosen to reproduce the magnetic moment and d-electron number for the bulk Fe and Cr.

The self-consistent calculations of the magnetic moments were performed for 20 configurations of SI and RI.

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The external magnetic field H shifts the energy of spin up states relatively spin down states on the value of 2 μ_BH. The calculations were performed for 39 values of H starting from the zero field. An initial configuration was chosen so that all Fe atoms have the same direction of the magnetic moments, whereas the Cr moments are ordered either along or opposite to the Fe moments with probability 0.5. The value $\mu_B H/\Gamma$, being a normalised magnetic field, changes in the following way: $0 \rightarrow -0.7 \rightarrow 0 \rightarrow 0.6 \rightarrow 0 \rightarrow 0.7$ with a step equal to 0.1. For each successive value of the magnetic field we used the self-consistent solution obtained for the previous field value as the initial configuration.

Table 1
Layer by layer distribution of the Cr atoms, Fe atoms, and empty sites for two monolayers of Cr coverage on the Fe substrate in the case of 'smooth' and 'rough' interface

Layer	Smooth interface			Rough interface		
	Cr	Fe	Emp	Cr	Fe	Emp
1	3	0	1277	24	1	1255
2	225	0	1055	178	19	1083
3	1051	2	227	496	156	628
4	1056	223	1	630	459	191
5	222	1058	0	487	768	25
6	3	1277	0	287	961	32
7	0	1280	0	166	1053	61
8	0	1280	0	112	1049	119
9	0	1280	0	85	1037	158
10	0	1280	0	54	1076	150
11	0	1280	0	38	1101	131
12	0	1280	0	0	1280	0

Fig. 1 shows the average projection on the parallel to applied magnetic field axis of the magnetic moments for the Fe and Cr atoms in one layer as a function of the applied field value. Fig. 1a and Fig. 1b corresponds, respectively, to the 4th and 5th layers of the SI (see Table 1). The number of the Fe and Cr atoms are given in the frame of the figures also. Hysteresis-like form of the curves reflects the plurality of the self-consistent solutions and their dependence on the initial configuration used for the self-consistent procedure. The shape of the loops essentially depends on the number of layers. It demonstrates that the moments in the different interface layers have a different response on the external perturbation, and consequently that the approach of an uniform

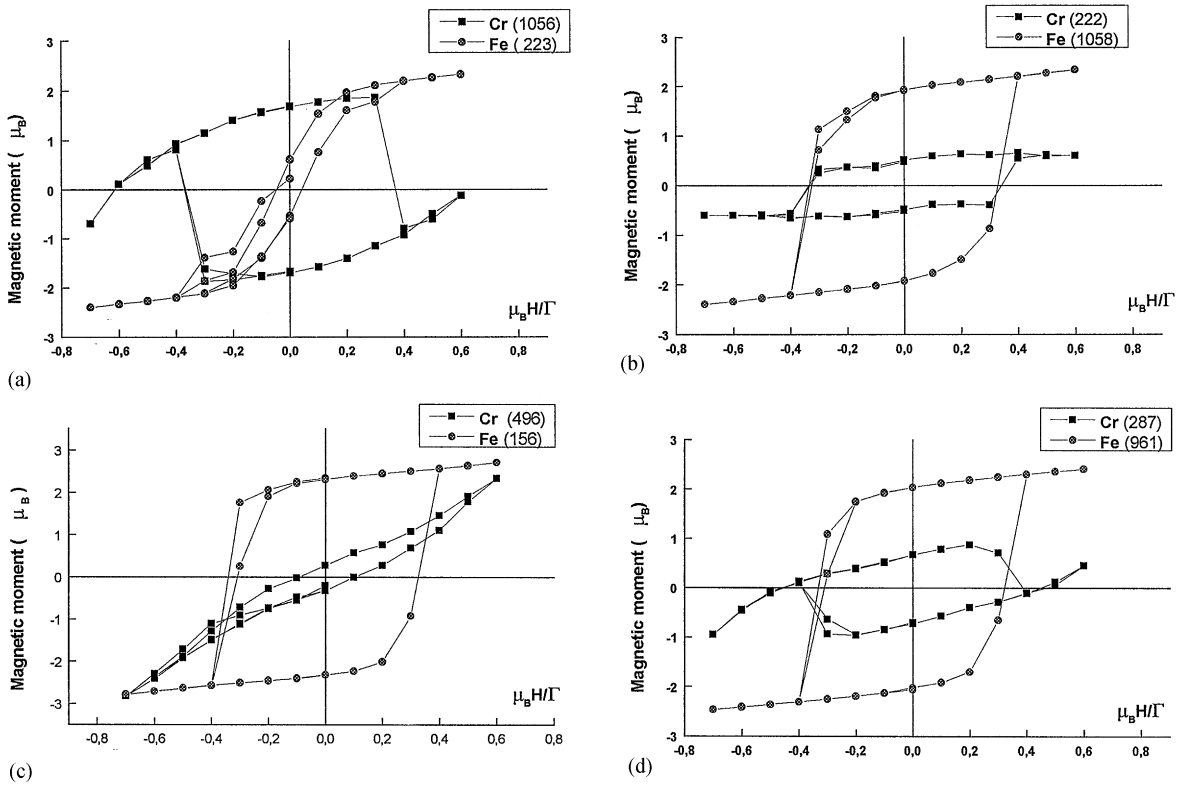

Fig. 1. Dependence of the average projection of the Cr and Fe magnetic moment in one layer on the parallel to the external magnetic fields axis versus the parameter $\mu_B H/\Gamma$. a – for the 4th layer SI, b – for the 5th layer SI, c – for the 3rd layer RI, d – for 6th layer RI.

magnetisation of Fe layers failed for these systems. The 4th layer (Fig. 1a) is filled mostly by the Cr atoms. Their magnetic moments are surface enhanced and antiferromagnetically (AF) coupled with the Fe substrate. When the magnetic field gives a spin-flop transition in the semi-infinite Fe (about $\mu_B H/\Gamma = \pm 0.4$) the magnetic moments of the Cr atoms change their direction on the opposite one. The Fe atoms in the 4th layer are much more flexible: the value and direction of the average Fe moment can be changed essentially by the relatively small external field. Next 5th layer (Fig. 1b) shows very stable moment of the Cr and Fe atoms, which stays almost unchanged till the spin-flop field. The magnetic moments directions of the Cr and Fe atoms coincide in this layer in spite of the AF coupling of Cr with respect to the Fe substrate.

Dependencies obtained for the RI (layers 3 and 6) are shown in Fig. 1c and Fig. 1d. The hysteresis loops for all Fe layers look similar to each other and the magnetic moments of the Fe atoms appear to be very stable. The moments of Cr, on contrary, show a different behaviour for the different layers. The Cr atoms transferred inside the Fe substrate (Fig. 1d) have the moments opposite to the Fe moments, and only slightly change up to the large fields. In the subsurface layers, where most of the atoms are also Cr ones, the magnetic moment can be easily reoriented (Fig. 1c): the average projection of the magnetic moment without the field close to zero, but in the presence of external field it can be enhanced up to 2 μ_B. These facts are in good agreement with out previous calculations of Cr overlayers on the Fe substrate [3], which show a large local moment but zero average.

Note, that all the calculations were performed within the collinear model. For the rough interfaces with a number of frustrations the canted spin structures are expected. Taking into account the possibility of the non-collinear states have to decrease essentially the value of spin-flop magnetic field.

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