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Noncollinear magnetism of Fe/Cr films and multilayers

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Abstract

The noncollinear magnetic structure of Fe overlayers on the stepped Cr substrate is calculated within the framework of a model Hamiltonian approach. Different noncollinear solutions are found by choosing the initial state for the self-consistency procedure. It is shown that for the stepped Fe/Cr interface the ground state is noncollinear and the distribution of magnetic moment directions is not uniform in both the Fe and Cr layers. The dependence of the angle between the average moment of the Fe overlayer and the average moment of different Cr layers on the thickness of Fe coverage is obtained.

Keywords: Noncollinear magnetism; Multilayers; Self-consistent solution; Stepped interface

During the last few years noncollinear (NC) magnetism of low-dimensional structures has been the subject of many investigations. In metallic magnetic multilayers, in particular in Fe/Cr sandwiches and superlattices, NC exchange coupling of magnetic layers was detected and different phenomenological models have been suggested for its explanation [1]. However, the microscopic calculation of NC magnetism in such systems, taking into account roughness and interdiffusion, appears to be a very complex problem and so far it has been performed only for several simple structures [2–4]. In this communication we report the results of self-consistent calculations of the magnetic order near an Fe/Cr interface for the Fe overlayer on stepped Cr substrate. The vector distribution of the magnetic moments on the Fe and Cr sites was obtained within a periodic Anderson model (PAM) using the "zero and pole" method for the density-of-states calculation [5,6]. PAM assumes the existence of two bands, one of which corresponds to the quasilocalized d-electrons and another to the itinerant s-electrons. The s–d interaction on site is presupposed to be stronger than d–s–d interaction between different sites. In this case in the model at first one should construct resonant d-states having a finite width due to the s–d interaction and then consider the d-electron hopping between different sites [7,8]. The Coulomb repulsion of the d-electrons on site was taken into account in the Hartree–Fock approximation, and the interaction between d-electrons localized on different sites was considered only inside the first coordination sphere of the atom under consideration. The self-consistent procedure calculated the values and directions of the magnetic moments on every site, locally corresponding to the minimum energy, while the other magnetic moments were fixed. The calculations were carried out for the Cr substrate covered by a different number of Fe layers with a stepped-like defect in the interface region. Fe and Cr atoms were placed at the sites of an ideal BCC lattice into the prism which includes 20 atomic layers with orientation (0 0 1) and 8×1 atoms in every layer. Periodic boundary conditions were used out of the prism. The bottom layer was filled by Cr atoms, and the value of the moments as well as their directions were kept fixed and equal to the bulk value for modeling of a semi-infinite substrate. The top layer was left empty, so that the previous layer appears to be the surface one. Most of the layers were filled by Fe or Cr atoms and only one interface layer contained an equal number of Cr (on sites 1,2,7,8) and Fe (on sites 3,4,5,6) atoms. Taking into account the periodic boundary conditions, such a structure

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corresponds to alternating up and down steps with a height of 1 monolayer at the Fe/Cr interface. The width of all steps is 4 atomic sites.

The NC self-consistent distribution of the moments essentially depends on the initial configuration which was chosen at the beginning of the iteration process. For Fe/Cr systems, in accordance with most available experimental data, all the moments lie in (0 0 1) plane, so that only one in-plane angle defines the direction of the moments. In our calculations the self-consistent magnetic moments obtained within a collinear model for the same system was used. Then the direction of the moments on the Fe atoms was rotated by an angle θ_0 relative to the Cr moments and this state was used as a start for the iteration procedure. The dependence of the energy of self-consistent solution ΔE (in arbitrary units) away from the corresponding value for the collinear model as a function of the angle θ_0 is shown in Fig. 1 for the 3.5 ML of Fe coverage on Cr. The same figure depicts also the angle θ between the average moment of the Fe overlayer and the average moment of the first layer after the interface layer, fully filled by the Cr atoms. The minimum energy for θ_0 is in the range 45–90°, so that the ground state for this system is an NC one. In the same interval of the initial angles θ_0 the values of self-consistent angles θ also stay almost constant. Taking into account that the minimum in the graphic $\Delta E(\theta_0)$ is in the indicated interval, to calculate the self-consistent NC state we used $\theta_0 = 90°$ as the initial angle. The dependence of the angle between magnetic moments of the Fe and Cr layers on Fe coverage is shown in Fig. 2, where solid squares, empty and solid circles correspond to the angles between the average moment in the Fe slab and in the Cr layers 1, 9 and 10 away from the interface, respectively. The angle between the average moment of the Fe slab and the magnetic moments in successive Cr layers (layers 9 and 10 in Fig. 2) is almost complemented to 180°, that point to the antiferromagnetic ordering of the Cr layers far enough from the interface. Angle between the moments of successive Cr layers is very close to 180°. The dependencies for all the curves of the same evenness of the Cr layers are very similar. For the small Fe coverage the oscillations of the angle take place, and for the thicker Fe overlayer we obtain almost 90°-coupling of Fe and Cr moments. Such behavior supports a conclusion about perpendicular ordering of Fe and Cr magnetic moments in the Fe/Cr/Fe sandwiches investigated by magnetic linear dichroism in core level photoemission [9]. Note also that near the stepped interface we obtain an NC moments' distribution, which is not uniform even inside the Fe slab. This fact has to be taken into account for interpretation of experiments on Fe/Cr multilayers, where the moment of Fe layers is usually characterized by single angle.

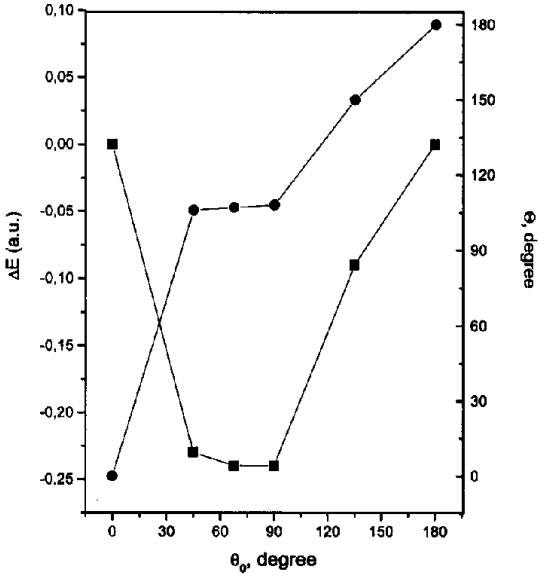

Fig. 1. Dependence of energy ΔE for the self-consistent solution counted from the collinear state energy (solid square) and of the angle θ between average magnetic moments in the Fe slab and in the first after the interface Cr layer (solid circles) on the initial angle θ_0, used in the iteration procedure.

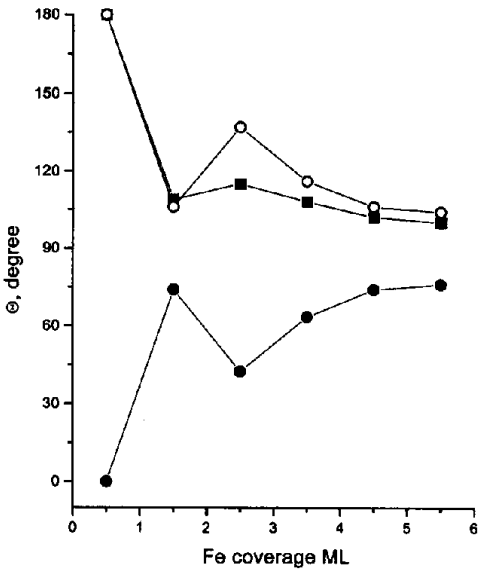

Fig. 2. Dependence of the angle θ between the average magnetic moment in Fe slab and in different Cr layers on the thickness of Fe overlayer. Solid squares, empty and solid circles correspond to the 1, 9 and 10 from the interface Cr layers, respectively.

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