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Noncollinear magnetic structure of Fe/Cr interfaces

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Abstract

A new method based on the periodic Anderson model is developed for a vector description of the magnetic moments near a stepped Fe/Cr interface. The method allows one to perform self-consistent calculations of local magnetic moment and d-electron numbers on a given atomic site for different orientations of the moment relative to the quantization axis. The self-consistent solution with minimal energy on a site under consideration is used to perform the calculation for the next step. In this approach the noncollinear magnetic structure for stepped Fe/Cr superlattices is obtained. The ground state is always noncollinear and the angle between magnetic moments of Fe layers depends on the thickness of the Cr and Fe layers.

Keywords: Noncollinear magnetism; Magnetic moment distribution; Self-consistent solution

Fe/Cr multilayers are the classical system, where noncollinear (NC) exchange coupling between Fe layers was originally discovered. Being a spin-density-wave system, Cr is very sensitive to interface roughness with other materials, and so far there is no general agreement about the physical mechanism responsible for the NC ordering in Fe/Cr superlattices. Experimental investigations performed by different groups on the Fe/Cr interface magnetism often lead to contradictory conclusions about its structure [1]. Calculations of magnetic order in collinear tight-binding models [2,3], that take into account roughness and interdiffusion demonstrate the existence of a number of self-consistent solutions close in energy, which are obtained by choosing different initial states in the iterative procedure. At the same time, existence of frustrations even for relatively simple stepped interfaces indicates that the ground state of real systems is most probably NC. Thus, development of a theory for a vector description of the interface magnetism is a fundamental problem for the true interpretation of experimental data.

In the present communication, we propose a new method for calculation of the values and directions of magnetic moments for the interface region of the Fe/Cr system. It is based on the periodic Anderson model (PAM) in the Hartree–Fock approximation and uses the real space recursion method [4]. For the description of NC magnetism we rewrite the PAM Hamiltonian in terms of spin quantization along a global z-axis, which is the same for all atoms. This leads to additional on-site hoppings with spin inversion, which depend on the angles between the magnetic moment and spin-quantization direction. Details of the calculations procedure based on the generalised 'zero and poles method' were reported in Ref. [4]. Here we dwell on the process of the self-consistent determination of the state with minimal energy and present the results of magnetic structure calculations of the Fe/Cr superlattices with stepped interfaces.

The problem of determining the state with minimal energy among different self-consistent solutions arises even in the collinear model. Most of the theories of NC

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structure either assume the symmetry of the ground state, as in the case of the systems with spiral magnetic structure [5,6], or start from non-self-consistent state and attain, using an iterative method, an output state that coincides with the input [7,8]. In this procedure the energy of the intermediate states is not taken into account and the final state is determined only by the initial configuration and the details of the iteration process. Actually the computer time necessary to converge the iterative procedure prohibits the computation of the structure for different initial states or change of the iteration procedure to compare the energy of different NC states. Thus we suggest another approach. The calculation starts from the self-consistent state obtained within the frame work of the collinear model. The directions of the moments on some sites are then modified so that the resulting NC state ceases to be self-consistent in a general case and in sequence the self-consistent d-electrons number and magnetic moment on every site are calculated for slightly different orientations of the moment on the site. If the angles, that determine the direction of magnetic moment on i-site, which are obtained on the nth step of the iteration process are $\theta_i = \theta_0$; $\varphi_i = \varphi_0$, then on the $(n+1)$th step we find the self-consistent magnetic moments for $\theta_i = \theta_0, \theta_0 \pm \Delta\theta$; $\varphi_i = \varphi_0, \varphi_i \pm \Delta\varphi$ and choose the state with minimal energy. The magnitude and direction of the surrounding magnetic moments are fixed during this procedure. However, such an iteration process for complex structures with a number of frustrations is often divergent. To make convergence more stable, we apply this procedure only to the atoms in one layer j_0, whereas the directions of the moments in all other layers $j \neq j_0$ were kept constant till all the moments and directions in the j_0-layer are converged. It is only after the directions of the moments on the j_0-layer have been fixed that the procedure starts on the next $j_0 + 1$ layer. In this case for every step of the iteration process we do not deviate much from the self-consistent state and obtain, as a result, a chain of states, each being different from the previous only by distribution of the directions of magnetic moments in one layer. The energy of these states, as a rule, decreases exponentially towards the minimal value. Note, however, that this procedure does not guarantee the convergence towards the ground state, but only to the state with a local minimum of the energy (minimal among the states that can be obtained from the given by small rotation of one individual moment).

Let us focus now on the results of the NC magnetic structure calculations performed for the Fe(1 0 0)/Cr(1 0 0) superlattices with stepped interfaces. The calculations were performed for $Cr_{n+1/2}Fe_{m+1/2}Cr_{n+1/2}Fe_{m+1/2}$ structures depicted in Fig. 1, with different number of layers n and m in Fe and Cr slabs. Periodic boundary conditions were used both in the plane and in the perpendicular directions. The regions with thickness of the Cr spacer equal to an even or odd number of atomic layers

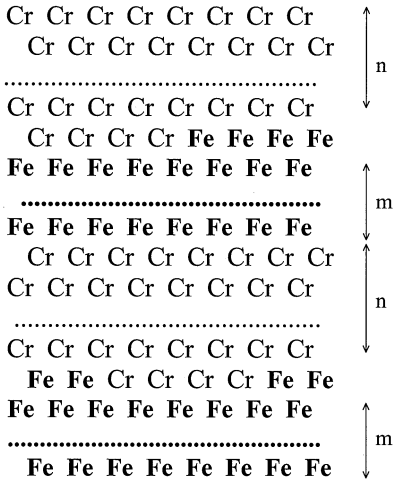

Fig. 1. $Cr_{n+1/2}/Fe_{m+1/2}/Cr_{n+1/2}/Fe_{m+1/2}$ superlattices with stepped interfaces.

alternate so that short-range (2 ML) oscillations of exchange coupling are almost suppressed in the first approach due to the stepped roughness. For the sake of simplicity the moments are fixed in the plane of the superlattices ($\varphi = 0$), in accordance with the last experimental investigations [1]. The distribution of in-plane magnetic moment directions, which are characterised by the angles θ_i and the moments M_i, were chosen in four different ways: (i) self-consistent collinear state, obtained in a collinear model with antiferromagnetically coupled Fe layers (AFCOL); (ii) self-consistent collinear state, obtained in a collinear model with ferromagnetically coupled Fe layers (FMCOL); (iii) non-self-consistent state, obtained from (i) by rotation of the Cr magnetic moment by 90° (AFNC); (iv) non-self-consistent state, obtained from (ii) by rotation of the Cr magnetic moment by 90° (FMNC). Fe moments for all initial states were chosen parallel and $\Delta\theta$ was accepted equal to $\pi/100$. The results of the calculations are shown in Table 1, where M_1 and M_2 are the modules of the average magnetic moments per Fe atom in the first and second iron slabs, Θ is the angle between these moments, ΔE is normalised (in units of the d-level width Γ [4]) energy of a given state counted from the state with maximal (among four calculated states) energy obtained for this structure. As is seen from the table, the collinear states in all cases correspond to a local minimum of the energy, and the ground state for the superlattices with stepped interface is NC. Despite the suppression by interface roughness of the short-range exchange coupling oscillations, they remain both in collinear and NC solutions. In the collinear case for the structure with even number n of full Cr layers, the state with $\Theta = 180°$ has less energy than with $\Theta = 0$. For odd n, the opposite result is obtained. The structures with odd and even n for NC solutions have essentially different self-consistent Θ. The state with minimal energy for

Table 1
Results of self-consistent calculations for stepped Fe(1 0 0)/Cr(1 0 0) superlattices

Structure	Initial state	M_1	M_2	Θ	ΔE
$Cr_{7.5}/Fe_{3.5}/Cr_{7.5}/Fe_{3.5}$	AFNC	1.90	1.91	82.2	− 2.121
$Cr_{7.5}/Fe_{3.5}/Cr_{7.5}/Fe_{3.5}$	FMNC	1.96	1.93	45.6	− 1.435
$Cr_{7.5}/Fe_{3.5}/Cr_{7.5}/Fe_{3.5}$	AFCOL	1.96	1.96	180	0
$Cr_{7.5}/Fe_{3.5}/Cr_{7.5}/Fe_{3.5}$	FMCOL	1.97	1.97	0	− 0.951
$Cr_{8.5}/Fe_{3.5}/Cr_{8.5}/Fe_{3.5}$	AFNC	1.90	1.91	132.0	− 1.085
$Cr_{8.5}/Fe_{3.5}/Cr_{8.5}/Fe_{3.5}$	FMNC	1.92	1.92	35.6	− 0.105
$Cr_{8.5}/Fe_{3.5}/Cr_{8.5}/Fe_{3.5}$	AFCOL	1.98	1.98	180	− 0.684
$Cr_{8.5}/Fe_{3.5}/Cr_{8.5}/Fe_{3.5}$	FMCOL	1.97	1.97	0	0
$Cr_{7.5}/Fe_{4.5}/Cr_{7.5}/Fe_{4.5}$	AFNC	1.96	1.97	93.0	− 2.080
$Cr_{7.5}/Fe_{4.5}/Cr_{7.5}/Fe_{4.5}$	FMNC	2.02	1.99	36.4	− 0.864
$Cr_{7.5}/Fe_{4.5}/Cr_{7.5}/Fe_{4.5}$	AFCOL	2.02	2.02	180	0
$Cr_{7.5}/Fe_{4.5}/Cr_{7.5}/Fe_{4.5}$	FMCOL	2.03	2.03	0	− 0.941
$Cr_{8.5}/Fe_{4.5}/Cr_{8.5}/Fe_{4.5}$	AFNC	1.95	1.98	134.4	− 1.386
$Cr_{8.5}/Fe_{4.5}/Cr_{8.5}/Fe_{4.5}$	FMNC	1.93	1.97	29.6	− 1.008
$Cr_{8.5}/Fe_{4.5}/Cr_{8.5}/Fe_{4.5}$	AFCOL	2.03	2.03	180	− 0.816
$Cr_{8.5}/Fe_{4.5}/Cr_{8.5}/Fe_{4.5}$	FMCOL	2.02	2.02	0	0
$Cr_{11.5}/Fe_{4.5}/Cr_{11.5}/Fe_{4.5}$	AFNC	2.01	1.99	97.2	− 0.878
$Cr_{11.5}/Fe_{4.5}/Cr_{11.5}/Fe_{4.5}$	FMNC	2.00	2.04	37.5	− 0.691
$Cr_{11.5}/Fe_{4.5}/Cr_{11.5}/Fe_{4.5}$	AFCOL	2.04	2.04	180	0
$Cr_{11.5}/Fe_{4.5}/Cr_{11.5}/Fe_{4.5}$	FMCOL	2.03	2.03	0	− 0.484

all considered structures is AFNC. For even and odd n, this state corresponds to the angles $\Theta = 130^\circ$–140° and 80°–100°, respectively. The decrease of the thickness of iron layers leads to a decrease in the difference between the angle of FMNC and AFNC states.

In summary, we developed a theory for the calculation of NC magnetism of Fe/Cr multilayers and performed the computation of the structure for superlattices with stepped interfaces. The ground state is NC and the angle between magnetic moments of Fe slabs depends on the thickness of Cr and Fe layers.

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