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Interface defects and formation of non-collinear magnetic ordering in Fe/Cr multilayers

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Abstract

Non-collinear magnetic structure of Fe/Cr multilayers was investigated within the framework of Periodic Anderson model (PAM) in mean field approximation for Coulomb repulsion on sites. Self-consistent calculations were performed for the superlattices with different step width at the interface. It is shown that due to frustration in the interface region the ground state corresponds to non-collinear orientation of magnetic moments near steps. This non-collinear ordering penetrates on a large distance from the interface both in Fe and Cr layers and leads to the non-collinear magnetic coupling between Fe layers through the Cr spacer. Angle between magnetic moments of Fe slabs depends strongly not only on the thickness of the Cr spacer but also on the interface structure at atomic scale. It is found that only very specific types of the interface defects with plural frustrations can give out-of-plane orientation of magnetic moments.

Keywords: Non-collinear magnetism; Rough interfaces; Fe/Cr multilayers

During the last decade, the multilayered systems were studied quite intensively because of their specific physical properties and possible technical applications. Large attention was given to the Fe/Cr multilayers where non-collinear (NC) coupling of Fe layers through Cr spacer was originally discovered. It is well established now that space defects such as steps at the interfaces, pinholes and embedded clusters are responsible for the biquadratic coupling in most of the metallic magnetic multilayers [1]. For Fe/Cr systems the magnetism of the Cr spacer plays an important role in the formation of NC order. For thickness less than the period of bulk Cr spin density wave NC magnetic structure is determined by the interface defects on the atomic scale. Taking into account that interdiffusion at Fe/Cr [2] and Cr/Fe [3] interfaces cannot be avoided it may be concluded that investigations relying size and shape of the interface defects from one side and formation of the NC magnetic ordering from another side is a problem of great importance.

In [4–6], we developed a method for the determination of the vector distribution of the magnetic moments in metallic multilayers with rough interfaces. It allows to calculate self-consistently the value and direction of magnetic moments localized on each atom in bcc lattice within Periodic Anderson model (PAM) in mean field approximation for Coulomb repulsion on site. The theory involves a very limited set of phenomenological parameters to determine the position of the d-level

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relatively to the Fermi level, the Coulomb repulsion on site, and the d-electron hopping between nearest neighbors. All these parameters are expressed in d-level width units, arising from the s–d interaction. Their values are fitted to reproduce the magnetic moments and the d-electron numbers in bulk ferromagnetic bcc iron and antiferromagnetic bcc chromium. The parameters have been used in many previous calculations [5–7] and they have given pertinent results. Calculations of the rough Fe/Cr interfaces within collinear PAM [7] shows that such a model can reproduce many characteristics of the real systems. In [5] it was shown that the NC coupling of Fe layers through the Cr spacer can be induced by the NC magnetic ordering of Cr arising around step edges due to frustration effect. Angles between the magnetic moments of the Fe slabs depend on the spacer thickness, although for superlattices with ideally smooth interface without intermixing the coupling stay collinear [5]. In the present communication, we consider stepped interface with different widths of Fe and Cr terraces and consequently with different ratio of Fe and Cr atoms in the mixed layer. Our main emphasis is on the link between interface defects and NC ordering in both Cr and Fe slabs.

Change of the Fe–Cr ratio in the interface layer leads to the structures with different numbers of Fe and Cr atoms in the supercell. To avoid this, we choose the system where the number of Fe (Cr) atoms are different in the first and second Fe (Cr) slabs, but the total number of Fe (Cr) atoms in the supercell and therefore the total d-electron number remains unchanged. Our supercell with 22 (0 0 1)-monolayers of Fe, Cr and Fe–Cr is shown in Fig. 1. Each layer is spatially homogeneous in x-direction and has a periodicity of 8 lattice constants in y-direction. From the 22 layers in cell 8 were filled by Fe atoms only (from 1st to 4th and from 12th to 15th), and 12 layers by Cr atoms only (from 6th to 11th and from 17th to 22th). Two layers (5th and 16th) contain both Fe and Cr. The mixed layers are parameterized by one integer number n, $0 \leqslant n \leqslant 8$: for the superlattice "$n$" the first n sites in the 5th layer were filled by Fe atoms and the remaining $8 - n$ sites by the Cr atoms. In the 16th layer Fe and Cr atoms were exchanged relatively to the 5th layer. The structure reported in Fig. 1

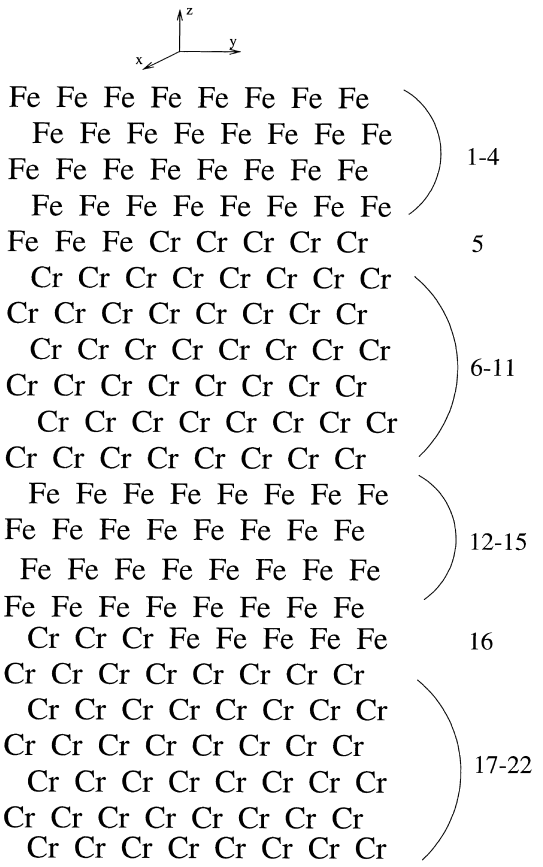

Fig. 1. Structure of supercell ($n = 3$) of 22 layers made of 4 Fe layers (1–4), mixed Fe–Cr layer (5), 6 Cr layers (6–11), 4 Fe layers (12–15), mixed Fe–Cr layer (16) and 6 Cr layers (17–22).

corresponds to $n = 3$. Due to the periodic boundary conditions, structures "n" and "$8 - n$" are physically equivalent. For $n = 0$ we have a superlattice with sharp interface but with different numbers of Fe and Cr layers in odd and even Fe and Cr slabs: $[Fe_4/Cr_7/Fe_5/Cr_6]$. If we remember that Fe–Cr and Cr–Cr couplings are antiferromagnetic [5,6] we can wait for this system NC coupling of Fe moments through the Cr spacer. On the contrary, from symmetry considerations, the superlattice "4" which has a chemical period of 11 ML should display collinear (ferro- or antiferro-) ordering of the average magnetic moments of Fe slabs, although ordering inside Fe slab as well as in Cr spacer can be NC.

Calculations of the vector distribution of the magnetic moments start from the self-consistent state, obtained in the collinear approach. As shown in [5,6] this state, is stable against infinitesimal rotation of individual magnetic moments on each specific site. To find NC solution we make large-scale perturbation of the magnetic moment's directions. In the first set of calculations we supposed that all the moments are ordered in the plane of the superlattice in accordance with most of the experimental data [8]. The direction of the moments on each site i is therefore determined by a single angle θ_i between magnetic moment and quantization axis. Starting from the collinear state we put $\theta = \pi/2$ on each Cr sites whereas θ_i remains equal to 0 or π on the Fe sites. After that the self-consistent calculations of the d-electron numbers and of the magnetic moments were performed consecutively on each site i for slightly different orientations (θ_i) of the moment on this site and the state with minimal energy was accepted for the next iteration. Details of this self-consistency procedure can be found elsewhere [5,6]. As a result, we obtained a sequence of self-consistent states with monotonically non-increasing energies. The energy of the final state was compared with the energy of the initial collinear state. For all the systems considered here, the energy of the NC state was found to be lower than that in the collinear one. However, this procedure does not guarantee the convergence to the ground state but only to the state with local minimum of energy among the states which can be obtained from given state by small rotation of one individual moment.

Fig. 2 presents layer by layer dependence of the angle Θ_i between average magnetic moment of the ith layer and the moment of the first Fe layer. Squares, diamonds, triangles up and down, crosses correspond to the "0", "1", "2", "3", "4" structures, respectively. A rotation of the magnetic moments take place both in Fe and Cr slabs. In the Fe slabs the average moments of the nearest layers are rotated from layer to layer by 5°–10°. Inside the Cr spacer the magnetic moments of the nearest layers are ordered almost antiparallel but twisted into spiral so that the moments of the next nearest neighbor Cr layers are rotated by 20°–30°. Similar

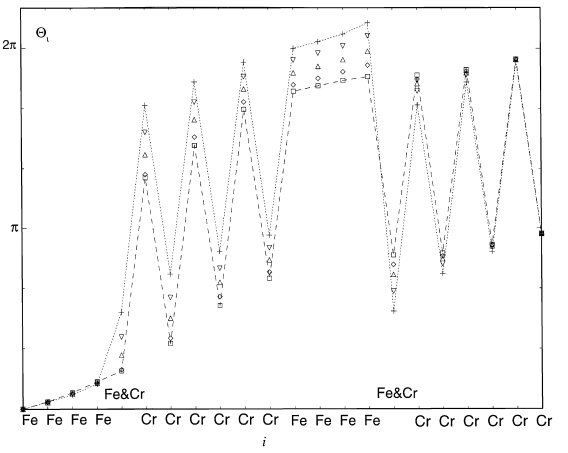

Fig. 2. Angle Θ_i between average magnetic moment in the ith layer (Fe, Fe & Cr, Cr) and the moment in the first Fe layer. Squares, diamonds, triangles up and down, crosses correspond to the structures with different width of Fe steps: structures "0", "1", "2", "3", "4", respectively. Lines are guide for the eye.

twisted structure in Cr spacer between two perfect Fe layers was already obtained in [9] within Hubbard-like tight binding model. However, in [9] angle between magnetic moments of Fe layers was keeped non-zero artificially but in our model with stepped interface NC structure self-organizes as a result of self-consistency and frustration effects.

Rotation of the magnetic moment in the mixed Fe–Cr layers depends essentially on the ratio between the number of Fe and Cr sites at the interface. At the first mixed layer, it is less than $\pi/2$ although it reaches 70° for the structure "4". The second mixed layer (16th layer) which contains in general more Cr atoms then Fe ones displays larger rotation angle between its average magnetic moment and direction of the moment in previous Fe layer (15th layer). Note that almost $\pi/2$-coupling of the Fe overlayer on stepped Cr substrate was obtained within the same model in [6] and detected in dichroism experiments [10,11].

The angle between the moments of the first and second Fe slabs is directly connected with the rotation angles between the moments of successive layers. In accordance with our symmetry considerations it is equal to 0 for the structure "4" where both stepped Fe interfaces have the same shape and maximal for the sharp interface (structure "0").

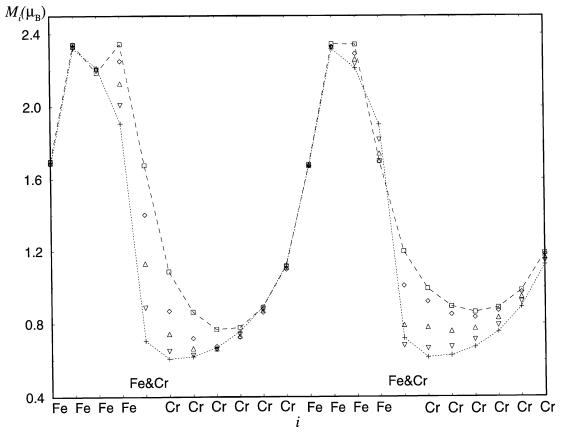

Fig. 3. Average magnetic moment per atom in the ith layer (Fe, Fe & Cr, Cr). Squares, diamonds, triangles up and down, crosses correspond to the structures "0", "1", "2", "3", "4", respectively. Lines are guide for the eye.

The layer-by-layer distribution of the average magnetic moments is shown in Fig. 3. For the ideally sharp interfaces the modulus of the average Fe magnetic moment decreases at the interface till 1.7 μ_B but, on the second from the interface layer an essential increase of the moment till 2.35 μ_B was detected. Similar behavior takes place in collinear approach [7]. Mössbauer measurements [8] show the same tendency for the hyperfine fields on Fe atoms at the first and second neighbors from the Fe/Cr interface layers. For the stepped interface average magnetic moments of mixed layers is much smaller and depends strongly on the Fe/Cr ratio at the interface. The modulus of the individual magnetic moments on Fe sites changes essentially less than the average moment. It means that the decrease of the average moment at the interface is predominantly connected with the change of the moment's orientations but not with the change of the their modulus on each site.

The distribution of the magnetic moments inside the Cr spacer in collinear and NC models prove to be significantly different. In collinear case frustrations suppress almost fully the magnetic moments on atoms around interface defects. After transition to the non-collinear state the sites with small magnetic moments on Cr atoms disappear and frustrations leads to the rotation of the moments. However step-like defects lead to a more fast decrease of the average moments versus distance from the interface and this decrease is maximal for an equal width of the Fe and Cr terraces.

We investigated also the possibility of an out-of-plane ordering of magnetic moments around the interface defects when the directions of the magnetic moments are determined by two angles: azimuth θ_i and polar ϕ_i. For this purpose we start from the NC state with $\theta_i \neq 0$ and $\phi_i = 0$ and then change angle ϕ_i from 0 to $\pi/2$ on some Cr sites near the interface. Iteration procedure performed previously for θ angle was extended by making small changes of both θ and ϕ angles and choosing for the next iteration the state with minimal energy.

NC out-of-plane ordering is stable only for interfaces having terrace width of Fe and Cr from 1 to 3 atoms. For such structures the out-of-plane states with a maximal angle $\phi \approx 20°$ was detected on some sites. At the same time, the average value of angle ϕ in the interface region did not exceed 5° and can hardly be detected experimentally.

In summary, we performed the calculation of vector distribution of magnetic moments in Fe/Cr superlattices with stepped interfaces and showed that NC ordering in Cr spacer can induce NC coupling of Fe slabs. Angle between the average magnetic moments of the Fe slabs depends not only on the thickness of the Cr spacer but also on the interface structure at the atomic scale.

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