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Pinhole defects in Fe/Cr trilayers

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Abstract

The distribution of magnetic moments in Fe/Cr/Fe sandwiches with pinhole defects has been studied using a model Hamiltonian approach. Self-consistent calculations were performed in the Hartree–Fock approximation for ideal smooth and rough interfaces generated by a special algorithm. For a sandwich structure of Fe antiferromagnetically coupled across a Cr spacer, the pinhole defects induce a non-zero magnetisation at zero external magnetic field. The value of the total magnetic moment appears, however, to be relatively small due to the effects of frustration which take place in the system. Fe atoms inside pinholes show different magnetic moments dependent on the number of Fe atoms among its nearest neighbours. The atoms at the border of the pinholes have magnetic moment smaller than the bulk value whereas moments of inner atoms are higher than in the bulk. The role of interface roughness and pinhole defects on the stability of these magnetic states has been investigated trough total-energy calculations.

Keywords: Interface magnetism; Interface roughness; Exchange coupling

Surface and interface defects which arise in low-dimensional magnetic systems (LDMS) due to the roughness and interdiffusion play a crucial role in their magnetic properties. The structure of multilayers is very sensitive to the quality of the substrate as well as to the conditions of the epitaxy process. However, the imperfectness in the space structure cannot be avoided at all [1]. That is why it is of interest and important from the applied point of view, to investigate different kinds of defects in order to clarify their influence on the magnetic properties of multilayers.

So far, most of the investigations of imperfect surfaces, overlayers and interfaces were concentrated on the step-like defects. The calculations which were performed within the Hubbard and the Periodic Anderson Model (HM and PAM) [2–4] show that distribution of the magnetic moments near the steps essentially differ from that of the ideal smooth surface. 'Topological antiferromagnetism' [2] which was obtained for the Cr stepped surfaces and the Fe overlayers on this surfaces made it possible to explain the discrepancy of different experiments with polarised electrons [5,6] as well as in situ magnetometer experiments which were performed on the samples with different roughness [7,8]. Step-like defects are responsible also for one of the mechanisms of non-collinear magnetic ordering in the multilayers [9]. Another kind of interface roughness was studied in Ref. [10], where the structure of the interface was modelled by special algorithm 'epitaxy' which keeps track of the descent of the Cr atoms dropped randomly on the Fe(001) surface. Such a modelling gives transparent picture of the transition from an oscillatory behaviour (for a relatively smooth interface) to a monotonous decrease (for a rough one) in the total magnetic moment of the sample [11,7].

In this paper we investigate pinhole structures in Fe/Cr multilayers. A pinhole is an iron bridge connecting two iron films through a chromium spacer. The existence of pinholes can explain some of the features of the magnetic behaviour, associated with the biquadratic exchange coupling [12]. Initially pinholes were introduced to explain non-zero magnetic moments for antiferromagnetically (AF) coupled bilayers [13]. In Ref. [14] a sandwich with pinhole defects described within a simple phenomenological model was used to determine the temperature behaviour of the total magnetic moment and the dependencies of all physical properties on the size of the pinholes. However this theory cannot be applied to the description of Fe/Cr systems, because the Cr spacer has its own magnetic structure which is strongly perturbed by the embedded Fe atoms. We use the PAM to obtain the distribution of magnetic moments for a Fe/Cr/Fe sandwich with Fe pinholes of different sizes. Localised magnetic moments of individual atoms are calculated self-consistently in the mean-field approximation by a recursive method in real

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space. These results are compared with those obtained for Fe clusters embedded in a Cr matrix [15,16].

The electronic structure of the sandwich $Fe_5/Cr_6/Fe_5$ with an ideal smooth interface as well as with a rough one determined by the algorithm 'epitaxy' A [10] is calculated. The epitaxy algorithm fills a selected prism with the atoms. Initially the prism bottom level is uniformly covered by Fe atoms. Then the Fe atoms are thrown on the top level of the prism with the random procedure. The algorithm follows their descending through empty sites until the sliding is blocked. Atoms are forced to slide onto available sites if it is empty with the equal probability. The Fe atoms are followed by the Cr ones and then the Fe atoms again. The number of Fe and Cr atoms was chosen the same as for the sandwich with ideal smooth interfaces. As a result we obtain the structure with rough Fe/Cr interfaces and rough top layers. It should be noted that roughness for this procedure does not exceed 2–3 layers.

The distribution of the magnetic moments was obtained for a 8 × 8 in plane structure with periodic boundary conditions. We have found solutions both with parallel and antiparallel ordering of the magnetisation in the Fe slabs. Due to the strong AF coupling of nearest Cr and Fe atoms and the AF order in the Cr spacer, first solution presents the frustration in the AF structure in the middle of the Cr slab. The solution with antiparallel magnetisation of the Fe layers appears to be energetically stable. Layer by layer average magnetic moments for both solutions are shown in Table 1 for the ideal smooth and for the rough interface. The layers from 1 to 5 and from 12 to 16 contain predominantly Fe atoms. For the rough interface there is an additional '0' layer. It consists of small islands of Fe atoms on the surface of the first layer. Correspondingly, the same number of empty sites are present in the first layer.

Table 1

Layer by layer average magnetic moment per site (in Bohr magnetons) in a given layer N in a sandwich without pinhole and with thin pinhole PH1, for smooth and rough interfaces. ↑↓ (↑↑) are for AF (FM) interlayer coupling between the Fe slabs. The last line gives the total magnetic moment of the sandwich for one site per plane

N	Without pinholes				With pinhole PH1			
	Smooth		Rough		Smooth		Rough	
	↑↓	↑↑	↑↓	↑↑	↑↓	↑↑	↑↓	↑↑
0	–	–	0.42	0.42	–	–	0.42	0.42
1	2.44	2.45	2.02	2.02	2.44	2.45	2.02	2.02
2	2.17	2.18	2.19	2.19	2.17	2.18	2.18	2.18
3	2.20	2.20	2.24	2.24	2.20	2.20	2.24	2.24
4	2.35	2.36	2.16	2.18	2.34	2.36	2.15	2.18
5	1.71	1.62	1.36	1.22	1.74	1.63	1.37	1.20
6	−1.23	−0.85	−0.27	0.10	−1.03	−0.57	−0.06	0.42
7	1.03	0.50	0.55	0.03	1.02	0.35	0.46	−0.23
8	−0.95	−0.16	−0.55	0.03	−0.98	0.06	−0.49	0.37
9	0.95	−0.16	0.56	−0.10	1.00	−0.29	0.56	−0.33
10	−1.03	0.50	−0.57	0.16	−1.09	0.68	−0.59	0.46
11	1.23	−0.85	0.31	−0.02	1.28	−0.93	0.32	−0.14
12	−1.71	1.62	−1.41	1.29	−1.71	1.66	−1.40	1.35
13	−2.35	2.36	−2.17	2.19	−2.34	2.36	−2.17	2.18
14	−2.20	2.20	−2.24	2.24	−2.20	2.20	−2.24	2.24
15	−2.17	2.18	−2.18	2.18	−2.17	2.18	−2.18	2.18
16	−2.44	2.45	−2.46	2.46	−2.44	2.45	−2.45	2.64
Σ	0	20.60	−0.04	20.83	0.23	20.97	0.14	21.22

Table 2

Layer by layer average magnetic moment per site (in Bohr magnetons) in a given layer N in a sandwich with an intermediate pinhole size PH2 and with a thick pinhole PH3, for smooth and rough interface. ↑↓ (↑↑) are for AF (FM) interlayer coupling between the Fe slabs. The last line gives the total magnetic moment of the sandwich for one site per plane

N	With pinhole PH2				With pinhole PH3			
	Smooth		Rough		Smooth		Rough	
	↑↓	↑↑	↑↓	↑↑	↑↓	↑↑	↑↓	↑↑
0	–	–	0.42	0.42	–	–	0.42	0.42
1	2.44	2.45	2.01	2.02	2.43	2.45	2.01	2.02
2	2.17	2.18	2.18	2.17	2.18	2.18	2.18	2.18
3	2.20	2.20	2.24	2.24	2.19	2.20	2.23	2.24
4	2.34	2.35	2.15	2.17	2.33	2.35	2.14	2.15
5	1.74	1.67	1.39	1.27	1.74	1.71	1.42	1.37
6	−1.02	−0.70	−0.15	0.22	−1.06	−0.87	−0.20	−0.02
7	1.08	0.62	0.67	0.19	1.16	0.86	0.83	0.64
8	−0.76	−0.07	−0.46	0.10	−0.80	−0.30	−0.56	−0.32
9	1.00	0.00	0.75	0.09	1.09	0.33	0.90	0.59
10	−0.83	0.55	−0.57	0.20	−0.87	0.28	−0.66	−0.23
11	1.26	−0.61	0.94	0.21	1.34	−0.25	1.00	0.62
12	−1.71	1.67	−1.20	1.30	−1.49	1.66	−1.23	1.24
13	−2.35	2.35	−2.17	2.18	−2.25	2.35	−2.16	2.18
14	−2.20	2.20	−2.24	1.24	−2.19	2.20	−2.23	2.24
15	−2.17	2.18	−2.18	2.18	−2.17	2.18	−2.17	2.18
16	−2.44	2.45	−2.45	2.46	−2.43	2.45	−2.44	2.45
Σ	0.75	21.49	1.33	21.66	1.20	21.78	1.48	21.95

For the first (1) and the last (16) layers one can see an enhancement of the magnetic moments whereas for the interface Fe layers (5 and 12) an essential decrease of the Fe moments takes place. This is in agreement with our previous calculations [2,10,17]. The Cr layers are AF ordered and the magnitude of the moments increases toward the interfaces. Note that for the solution with rough interface we obtained an extremely small total magnetic moment for the AF coupled sandwich. The averaged magnetic moment per site in the layer for sandwiches with pinholes are presented in Tables 1 and 2. Because we are not aware of any detailed chemical structure of the Fe/Cr sandwiches we consider three different sizes of pinholes. The number of the Fe atoms in odd and in even Cr layer due to the pinhole existence was taken correspondingly 1 and 4 for PH1, 5 and 4 for PH2, 9 and 4 for PH3 (see Fig. 1a–1c). Fig. 1 shows four successive layers of the sand-

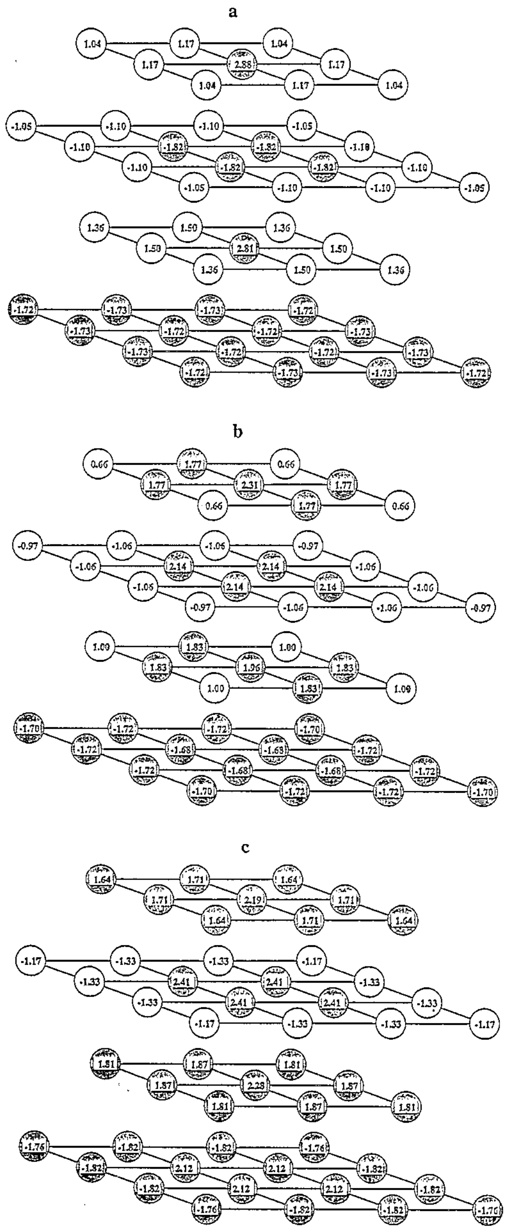

Fig. 1. Distribution of the magnetic moments (in Bohr magnetons) of the Fe and Cr atoms around pinholes. Grey and white circles depict the Fe and Cr atoms, respectively. The bottom layer belongs to the Fe slab. (a) PH1 – thin pinhole with a number of iron atoms 1 for odd, 4 for even layers; (b) PH2 – pinhole of an intermediate size with the number of iron atoms 5 for odd, 4 for even layers; (c) PH3 – thick pinhole with a number of iron atoms 9 for odd, 4 for even layers.

wich with pinholes connecting two AF coupled Fe slabs with smooth interfaces. Grey and white circles depict Fe and Cr atoms respectively. The bottom layer in the figures belongs to the Fe slab (12th in Tables 1 and 2). The other layers contain the Fe atoms embedded into the Cr spacer.

It is well-known that Fe atoms in a bcc lattice prefer ferromagnetic (FM) ordering with the nearest other Fe atoms. For the structure under consideration there is frustration due to the AF coupling in the sandwich. It leads to the spin-flop transition inside or in the neighbourhood of the pinhole. How this transition depends on the thickness of the pinhole can be seen from Fig. 1a–1c. For the thin pinholes (PH1 – Fig. 1a) every odd layer contains only one Fe atom. It appears to be non-sufficient for a FM arrangement of the Fe atoms. As a result their magnetic moments follow the Cr AF structure and change their direction every next layer. Note that for the solution with parallel magnetisation in Fe slabs there is no such AF structure in the pinhole PH1, but some Cr atoms around pinhole change their magnetic moment opposite to Cr moments in this layer.

For the pinhole PH2 with an intermediate size (Fig. 1b) a spin-flop transition takes place between the 12th and the 11th layers. Thus, the magnitude of the magnetic moments of the Fe atoms decrease essentially. Note that the value of the magnetic moments of the Fe atoms having mostly nearest Cr neighbours, appears smaller then in the bulk. The moments of the atoms inside the pinhole, which are surrounded by Fe atoms exceed the bulk value. This is similar to the results obtained for small Fe clusters embedded in a Cr matrix [15,16] and with the behaviour of the interface moments in the superlattice Fe/Cr [17]. For the thick pinhole PH3, depicted on Fig. 1c, the influence of the top iron slab is so strong that it perturbs the Fe atoms in the bottom slab: magnetic moments near the base of the pinhole change their direction from AF to FM relatively the top Fe layer. As a result, in the sandwich with relatively thick pinholes regions with ferromagnetic and antiferromagnetic interlayer coupling, can change their physical characteristics This type of behaviour was observed in annealed Fe/Cr multilayers using polarised neutron technique [18].

The magnitude of the magnetic moments of the Cr atoms around pinholes increases. Due to the AF coupling of nearest Fe and Cr atoms it leads to the screening of the pinholes magnetic moment and the decrease of the total magnetic moment of the AF coupled sandwich. Thus, the moment of the sample at zero field appears to be relatively small despite of the FM ordering inside pinhole. Its value, however, essentially exceed that due to interface roughness in our model. For the sandwich with rough interfaces the deviation of the total magnetic moment prove to be greater than for the smooth one because of the interference of pinhole effects and random roughness. However one can see an increase of the total magnetic moment with pinhole size in both cases.

The calculation of the total energy shows that for smooth interface and for weakly rough ones considered here, pinholes cannot change the ground state of the sandwich and the type of Fe slabs ordering from AF to FM. It can happen, however for more rougher interfaces.

Note that the weak roughness, which in our case does not exceed two layers, leads to a decrease of the magnitude of the Cr atom's magnetic moment around pinholes. So in the case of essential roughness pinholes can suppress AF ordering in the spacer. In any case pinholes have to reduce saturation magnetic field as well as giant magnetoresistance, which is proportional to the amount of AF coupled domains. So these defects can be one of the reason of the behaviour of Fe/Cr multilayers after annealing [18].

In summary, we have calculated the distribution of the magnetic moments in the sandwich structure with pinhole defects. For Fe slab AF coupled across a Cr spacer sandwich we obtain a non-zero total magnetic moment. The distribution of the moments inside pinhole is similar to the Fe clusters embedded into a Cr matrix. Thick pinholes can lead to the creation of domains in the Fe slab with opposite magnetisation.

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