Fe clusters near the surface and interface in the FeCr systems

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Abstract

Magnetic and electronic properties of Fe_N clusters embedded in antiferromagnetic BCC Cr near the sample surface as well as near the Fe/Cr interface have been studied within the framework of the periodic Anderson model. A distribution of the magnetic moments is determined self-consistently in the mean-field approximation taking into account the d–d-interaction in the first coordinate sphere of atoms. For all the investigated systems several magnetic configurations are found, and the energy of all configurations is calculated. The magnetic structure dependence on the size of clusters as well as on the spatial nonhomogeneity caused by surface or interface is investigated.

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1. Introduction

Modern development of technology in creation of the artificial low-dimensional magnetic structures causes a considerable interest in the theoretical studying of the properties of imperfect systems with broken space symmetry.

Of special interest is the investigation of the rough surfaces and interfaces because such interfaces are much easy to obtain than a perfectly smooth one and, therefore, they are more promising for any future applications. It is worthwhile to note that

a number of phenomena in the artificially made systems depend crucially on a perturbation of space symmetry, and consequently such structural defects have to be taken into account in all theoretical schemes which pretend to describe real experiments.

In recent years, the magnetic multilayers have attracted much attention because of a variety of interesting physical phenomena such as antiferromagnetic exchange coupling and giant magnetoresistance [1, 2] which were discovered in these systems.

One of the most challenging systems, which display a number of unusual properties, is artificially made multilayers on the FeCr base. Roughness of the surfaces as well as interfaces appears to be

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extremely important to understand the physical nature of its properties. For example, a long-range period of exchange coupling oscillations in the Fe/Cr superlattices can be observed only if the short-range oscillations are suppressed by the interface roughness [3]. It causes the considerable interest in the theoretical description of imperfectness of the multilayer structure. Ab initio theories cannot properly describe such complex systems, so that a model Hamiltonian approach, such as the Hubbard model (HM) and the periodic Anderson model (PAM), is used for this purpose.

Within the framework of the HM the distribution of magnetic moments on the stepped Cr surface has been calculated in Ref. [4]. These results allowed to explain the apparently contradictory observations which had been obtained by spin-resolved and angle-and-energy-resolved photoemission [5, 6]. In Ref. [7] the magnetic properties of Fe overlayers on Cr (0 0 1) were calculated taking into account the roughness of interface.

PAM has been used to calculate the magnetic properties of impurity Cr atoms both in the Fe bulk and near the surface [8]. Using a random modelling of the epitaxial process, a reasonable explanation of Turtur and Bayreuther magnetometer experiments [9] was proposed [10]. Note that the results obtained for the same system with the different tight binding Hamiltonians often appear to be in a qualitative agreement [11].

In this work, within the PAM we have calculated the magnetic and electronic properties of Fe_N clusters ($N = 15, 9, 2$) embedded near Cr surface and Fe/Cr interface. Such clusters often exist in the real multilayer systems or can arise there during the annealing process. Similar calculations were performed in Ref. [12] for the isolated Fe_N clusters and in Ref. [13] for substitution cluster impurities in bulk Cr in the HM.

2. Theory

The calculations of the electronic and magnetic structure of Fe clusters in the Cr matrix were performed within PAM in the mean-field approximation by real-space method [8, 10].

We assume that energy spectrum for such a system is described by two bands which correspond to the 3d and 4s electrons. The Hamiltonian of the system in the mean-field approximation reads

$$H = \sum_{i,\alpha} \epsilon_{i\alpha} \hat{d}_{i\alpha}^{+} \hat{d}_{i\alpha} + \sum_{\alpha, i \neq j} t_{ij} \hat{d}_{i\alpha}^{+} \hat{d}_{j\alpha} + \sum_{k\alpha} \epsilon_{k} \hat{c}_{k\alpha}^{+} \hat{c}_{k\alpha}$$
$$+ \sum_{\alpha, ki} V_{ki} \hat{c}_{k\alpha}^{+} \hat{d}_{i\alpha} + \text{h.c.} \qquad (1)$$

Here $\hat{d}_{i\alpha}^{+}$ ($\hat{d}_{i\alpha}$) and $\hat{c}_{k\alpha}^{+}$ ($\hat{c}_{k\alpha}$) refer to the creation (annihilation) operators of d-electrons with spin α on the atomic site i and of s(p)-electrons with quasi-momentum k and spin α, respectively. $\epsilon_{i\alpha}$ and ϵ_{k} are the energies of these electrons. The hopping parameters t_{ij} and s–d-hybridisation potential V_{ki} are taken to be spin-independent.

Equation for the Green function G_{ij}^{α} of d-subsystem has a form:

$$(\omega - E_{i,\alpha}) G_{ij}^{\alpha} - \sum_{i'} V_{ii'} G_{i'j}^{\alpha} = \delta_{ij}. \qquad (2)$$

The energies of d-electrons $E_{i,\alpha}$ as well as hopping parameters $V_{i,i'}$ contain the parts determined by s–d-hybridisation:

$$E_{i,\alpha} = \epsilon_{i,\alpha} + \sum_{k} \frac{V_{ik} V_{ki}}{\omega - E_{k}}, \qquad (3)$$

$$V_{ii'} = t_{ii'} + \sum_{k} \frac{V_{ik} V_{ki'}}{\omega - \epsilon_{k}}. \qquad (4)$$

Note that the energies $E_{i,\alpha}$ have an imaginary part, which is determined by s–d interaction:

$$\Gamma_{i} = \text{Im} \sum_{k} \frac{V_{ik} V_{ki}}{\omega - \epsilon_{k}}. \qquad (5)$$

The PAM presuppose that the coupling of s and d-electrons on site is comparatively strong, while the coupling between d-electrons on different sites due to d–s–d interaction is relatively small. In this case, one should first construct resonant d-states having finite width Γ and then consider the interaction between different atoms.

We assume that the quantities Γ_i to be independent of site i and treat them as parameters of the model. The iterative solution of the equations for the d-electron Green function we present in the

following form:

$$G^{\alpha}_{ii'} = \frac{1}{\omega - E_{i,\alpha}}\left[\delta_{ii'} + \frac{V_{ii'}}{\omega - E_{i',\alpha}} \right.$$
$$\left. + \sum_j \frac{V_{ij}V_{ji'}}{(\omega - E_{j,\alpha})(\omega - E_{i',\alpha})} + \cdots \right]. \quad (6)$$

For the diagonal matrix elements G^{α}_{ij} one can obtain

$$G^{\alpha}_{ii} = (\omega - E_{i,\alpha} - \Sigma_{i,\alpha})^{-1}. \quad (7)$$

Here the mass-operator $\Sigma_{i,\alpha}$ is determined by the expression

$$\Sigma_{i,\alpha} = \sum_j \frac{V_{ij}V_{ji}}{\omega - E_{i,\alpha}} + \sum_{j,l} \frac{V_{ij}V_{jl}V_{li}}{(\omega - E_{j,a})(\omega - E_{l,a})} + \cdots. \quad (8)$$

The summation in Eq. (8) is carried out over all the transitions paths which start and finish on the ith site and, moreover, do not go through it any more. We calculate the function $\Sigma_{i,\alpha}$ by taking into account a certain set of atoms m_i associated with the ith site and considering only the transitions through the atoms of this set. In this case the self-energy function $\Sigma_{i,\alpha}$ can be represented as follows:

$$\Sigma_{i,\alpha} = \sum_{j \in m_i} V_{ij}S^{\alpha}_{ji}, \quad (9)$$

where S^{α}_{ji} are the contributions from all the paths which start from the jth site and finish at the ith site. We determine that the matrix S^{α}_{ji} obeys the following set of equations:

$$(\omega - E_{j,\alpha})S^{\alpha}_{ji} = V_{ji} + \sum_{l \in m_i} V_{jl}S^{\alpha}_{li}. \quad (10)$$

In what follows, we restrict the set of m_i to the first coordination sphere of the site under consideration. In this case influence of second neighbors can be only indirect due to change of d-electron energy for the atom from the first coordinate sphere. Note, however, that calculations of magnetic moment distribution which were performed in this approach and within HM, taking into account transitions between first and second neighbors, gave close re-

sults for stepped surfaces of Fe and Cr as well as for monolayer of Fe(Cr) on stepped Cr(Fe) substrate [11].

The d-electron state occupation numbers are given by the expression:

$$N^{\alpha}_i = 5n^{\alpha}_i = -\frac{5}{\pi}\int d\omega f(\omega)\, \text{Im}\, G^{\alpha}_{ii}(\omega - i0), \quad (11)$$

where $f(\omega)$ is the Fermi–Dirac function.

For the self-consistency procedure we will use the simplest condition which has already appeared in the Hartree–Fock approach

$$E_{i,\alpha} = E_{0i} + U_i n^{-\alpha}_i, \quad (12)$$

where E_{0i} and U_i are parameters of the model. The set of Eqs. (7)–(12) allows us to calculate the quantities N^{α}_i, $E_{i,\alpha}$ self-consistently.

The theory involves a very restricted set of phenomenological parameters which can be determined via calculations of the bulk Fe and Cr properties (the number of d-electrons per atom $N_{Fe} = 7.0$, $N_{Cr} = 5.0$, and the magnetic moments $M_{Fe} = 2.2\,\mu_B$ for ferromagnetic ordering, $M_{Cr} = 0.6\,\mu_B$ for antiferromagnetic ordering). These parameters are the initial energy of d-level E_{0i}, Coulomb integral U_i, 'hopping' parameter V_i (which we consider to be non-zero only for nearest neighbors) and the level width Γ. It is convenient to use the dimensionless variables

$$x_i = \frac{E_{0i} - E_F}{\Gamma}; \qquad y_i = \frac{U_i}{\Gamma}; \qquad z_i = \frac{V_i}{\Gamma}.$$

Although all these values for every element cannot be found in a unique manner (there are three parameters and only two conditions for their determination), the range of their change appears to be very restricted, and the resulting distribution of magnetic moments is not sensitive to the small variations of parameters.

As an initial approximation for the self-consistent calculation, we use the populations of the electron states which correspond to the pure ferromagnetic (FM) Fe and antiferromagnetic (AF) Cr. At initial stage, it was possible to choose the magnetic moment of Cr and Fe atoms at every site to be both up and down. Self-consistent solutions, as a rule, depend on the initial spin configuration

[14]. However, in some cases, for example, for one impurity atom in the bulk metal, there is a unique self-consistent solution independent of the initial state [8].

The mass operator in our approach is determined by the atoms in the first coordination sphere of the atom under consideration. The Fermi level ϵ_F, and consequently the parameter x_i, was chosen so that the total d-electrons number in the sample being conserved equal to the corresponding number in the bulk. The calculations were performed using two different approximations:

(i) Local electroneutrality (LE). In this case the occupation numbers of matrix atoms, located on the Fe cluster's interface further apart of the third nearest neighbors, were taken to be the same as in pure Cr. The self-consistency procedure and Fermi level shift have been introduced only for the cluster's atoms and matrix atoms from two neighbouring coordination spheres around cluster. Such approximation was used to calculate the magnetic structure for the Cr clusters in Fe matrix [8] and Fe clusters in Cr matrix [13].

(ii) Global electroneutrality (GE). The self-consistency procedure is expanded on all the atoms of the sample. In our calculations we put all the sample's atoms into the prism. The base of the prism comprises 8×8 elementary cells. Its height is 18 levels. Outside of the prism we periodically repeat this structure. Here, the shift of the Fermi level for a self-consistent solution depends on the occupation number of all atoms.

The second algorithm was much more time consuming. However, for the calculation of spatially nonhomogeneous system with lengthy heterogeneity, such as surface or interface, it can be required, because the perturbation of magnetic moments penetrates on the large distance.

To find the ground magnetic state for embedded clusters, we calculated the energy of d-electrons. For electrons localized on the site i we have

$$\epsilon_i = 5 \sum_\alpha \int_{-\infty}^{\epsilon_F} d\omega \, \omega \rho_i^\alpha(\omega) - 5 U n_i^\uparrow n_i^\downarrow,$$

where $\rho_i^\alpha(\omega)$ is the density of states for the electrons on site i with spin projection α. Total energy can be obtained as the sum over all the sites. Note that when we use our dimensionless parameters, the total energy also will be dimensionless (in Γ units).

3. Results and discussion

We consider the Fe clusters embedded into the Cr matrix. The surface of the sample or Fe/Cr interface is taken to be ideally smooth with orientation (0 0 1). Bulk Cr below the Neél temperature $T_N = 311$ K orders as an incommensurable spin density wave (SDW) antiferromagnet with the wave vector Q along the (0 0 1) direction, determined by the nesting. Wavelength of SDW is about 21 lattice constant and as a first approach we will consider the bulk Cr as being possessed of simple AF structure, so that the (0 0 1) planes contain atoms of only one spin direction. Consequently, the (0 0 1) surface is expected to have ferromagnetic order. In Fig. 1 are shown three clusters Fe_2, Fe_9, Fe_{15}. Atoms in the equivalent positions are denoted by the equal numbers.

For the Fe clusters, embedded on the large distance from the surface, we obtained different solutions depending on the initial state of the self-consistency procedure. The magnetic moments and the number of particles for different Fe atoms in cluster Fe_{15} and nearest Cr atoms are given in Table 1.

FM1 and FM2 in this table correspond to the FM ordering of magnetic moments in the Fe cluster. For FM1 the magnetic moment of the central atom 1 in Fig. 1c points the parallel direction to the magnetic moments of the Cr atoms in the same (0 0 1) layer. For FM2-solution these magnetic moments are oriented antiparallel. Note that the solution which was found in Ref. [13] for the Fe_{15} cluster, corresponds to the FM1-state. The energy of this state in our calculation appears to be more than for FM2-solution. However, such a state can exist as a metastable one. As it is evident from the table, the calculations in the GE and LE approximations give close results for the FM clusters.

Third solution shows AF ordering in the cluster that repeats a layered antiferromagnetism in the Cr matrix. The energy of this state turns out to be less than the energy for both FM states. This solution
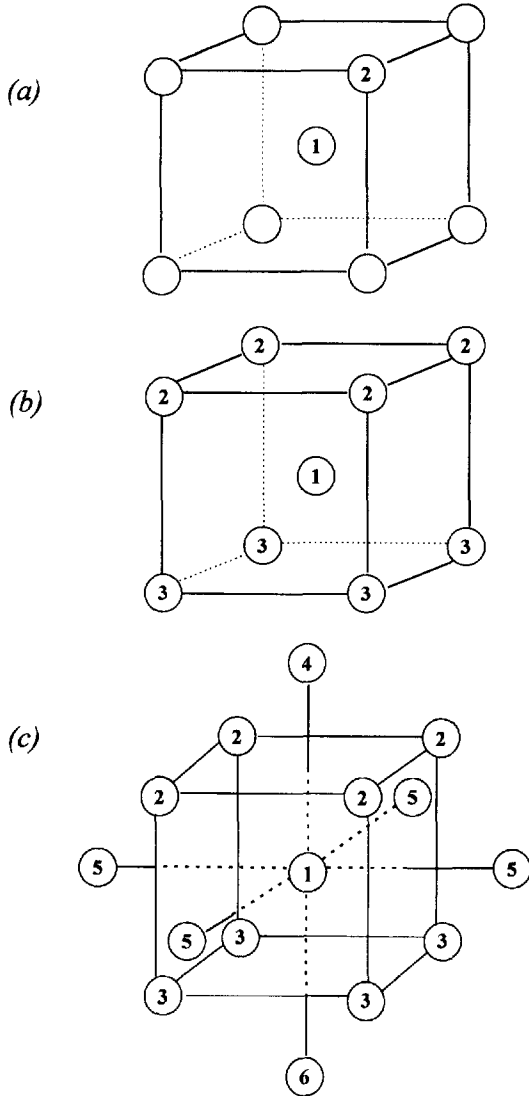
Fig. 1. Iron clusters (a) – Fe_2, (b) – Fe_9, (c) – Fe_{15}. Different ciphers denote atoms in nonequivalent positions.

gives large deviations of the magnetic moments and of the number of d-electrons per site with the same correspondent values in the bulk α-Fe. The results of calculations in the GE and LE approximations differ here more than for the FM solution. It is connected with a charge transferring on a large distance from the cluster. All atoms in the cluster and in the Cr atoms surrounded it have less number of electrons than in the bulk. So, the region

around the cluster will have positive charge which gives an additional electrostatic contribution to the total energy. This contribution was not taken into account in our calculations of energy. Such a large charge transfer can lead to the instability of AF state.

Similar magnetic structure was obtained for the Fe_9 cluster (Table 2), but in this case, only one FM solution exists. The second FM initial state converges to the AF solution after the procedure of self-consistency.

For all self-consistent solutions the central Fe atom posses a larger magnetic moment than in the bulk, whereas the interface atom's magnetic moments are less than the bulk value. Note that the calculations of Fe_3/Cr_n superlattice magnetic structure show the increase of magnetic moments for the central Fe layer and decrease of them for the interface layers [8, 15].

For the Fe_2 cluster, where there are no inner Fe atoms, we found only AF solution with the magnetic moments ± 1.41 μ_B. Magnitudes of magnetic moments for the Cr atoms around cluster appears to be slightly increased but not more then 0.1 μ_B.

Existence of different magnetic solutions for relatively large clusters is connected with frustration effects. It is well known, that for the nearest Fe atoms a parallel alignment of magnetic moments is preferable but neighbouring Fe and Cr atoms usually have antiparallel magnetic moments [4, 11]. For a small cluster the FM coupling between nearest Fe atoms is not enough to arrange the magnetic moments in a parallel way and their magnetic structure repeats the structure of AF Cr. However, the greater the cluster, the greater is the role of FM interaction between Fe atoms, and this interaction stabilises the FM ordering inside of the cluster. For large clusters with complex shape one can expect a number of different self-consistent solutions with a breakdown of FM ordering for the interface atoms having the less Fe atoms among neighbours.

Smooth surface or interface introduces an additional layered structure, which coincides in our case with AF layered structure of the bulk Cr. Influence of the surface is superimposed on the cluster's magnetic structure. The number of nearest neighbour for surface atoms is less than for bulk one. It leads to the effective shrinking of the d-band and

Table 1
The magnetic moments (M) and the number of d-electrons per atom (N) for Fe_{15} cluster and nearest Cr atoms far from the surface

Atom's number in the cluster	Global electroneutrality						Local electroneutrality					
	FM1		FM2		AFM		FM1		FM2		AFM	
	M	N	M	N	M	N	M	N	M	N	M	N
1	2.62	6.71	2.49	6.83	2.97	6.09	2.58	6.76	2.48	6.86	2.89	6.23
2, 3	1.36	7.03	1.91	6.83	− 1.86	6.67	1.41	7.05	1.84	6.89	− 1.58	6.84
4, 5, 6	1.95	6.80	1.41	7.01	1.83	6.69	1.91	6.84	1.52	7.03	1.63	6.82
Cr: 3rd sphere	0.45	4.95	− 0.77	4.92	0.85	4.91	0.47	5.01	− 0.72	4.98	− 0.72	5.02

Table 2
The magnetic moments (M) and the number of d-electrons per atom (N) for Fe_9 cluster and nearest Cr atoms far from the surface

Atom's number in the cluster	Global electroneutrality				Local electroneutrality			
	FM		AFM		FM		AFM	
	M	N	M	N	M	N	M	N
1	2.65	6.71	3.00	6.11	2.65	6.72	2.96	6.21
2, 3	1.51	6.86	− 1.54	6.81	1.38	6.93	− 1.36	6.90
Cr: 2nd sphere	− 0.96	4.79	0.95	4.79	− 0.86	4.86	0.84	4.87
Cr: 3rd sphere	− 0.78	4.91	0.78	4.91	− 0.71	4.98	0.70	4.99

increasing of the subsurface magnetic moments [6, 8, 15]. The same behaviour takes place for cluster's atoms.

The magnetic moments and the number of electrons localised on the Fe atoms for cluster Fe_{15} touching the sample surface and located on the next layer after the surface, are given in Table 3. In the same table the data for the Cr atoms of third neighbours of the central Fe atom, but placed on the different distances on the surface are presented.

For all solutions, the magnetic moments increase toward the centre of cluster as well as toward the surface of the sample. The maximum magnetic moments have the surface atoms (4). Magnetic moment of the central atom (1) is also enhanced relatively by the bulk Fe, and the magnetic moments of the surface Cr atoms around the Fe island (2.4 μ_B) turn out to be more than for the vicinal Cr surface (2.13 μ_B).

The surface imposes AF layer structure on the iron clusters. Really, in the presence of the surface, the FM1 solution is no longer FM one. It contains four atoms with opposite spin in the second layer for the cluster touching the surface and in the third layer for the cluster under the surface. Energy for the second FM solution FM2 is also increased in comparison with that for the AFM solution. Note that AF structure of the cluster can be destroyed by surface roughness of the real sample. In this case, the distribution of magnetic moments in the cluster will depend on the local geometry of the surface.

Cluster Fe_9 has a magnetic structure similar to Fe_{15} (Table 4). Magnetic moment of the central Fe atom (1) for both cases appears to be very close, whereas the Fe atoms (2) and (3) at the cluster boundary for Fe_9 turn out to be less than for Fe_{15}. It can be explained by less number of nearest neighbours Fe atoms for smaller cluster.

Table 3
The magnetic moments (M) and the number of d-electrons per atom (N) for Fe_{15} cluster and nearest Cr atoms in the presence of the surface

Atom's number in the cluster	Fe_{15} touching surface						Fe_{15} one layer from the surface					
	FM1		FM2		AFM		FM1		FM2		AFM	
	M	N	M	N	M	N	M	N	M	N	M	N
1	2.38	6.59	− 2.45	6.87	2.96	6.07	− 2.41	6.58	2.46	6.86	− 2.97	6.09
2	− 2.42	6.43	− 2.19	6.74	− 2.44	6.42	2.18	6.54	2.09	6.76	2.21	6.53
3	1.42	7.03	− 2.00	6.79	− 1.97	6.64	− 1.44	7.02	1.97	6.80	1.94	6.65
4	3.29	6.07	− 2.69	6.76	3.28	6.08	− 2.54	6.37	1.52	7.11	− 2.53	6.37
5	2.02	6.69	− 1.19	7.09	2.10	6.58	− 1.95	6.72	1.27	7.06	− 2.01	6.62
6	1.96	6.80	− 1.35	7.03	1.87	6.68	− 1.96	6.81	1.37	7.03	− 1.86	6.68
Cr: 3rd sphere	1 layer		1 layer		1 layer		2 layer		2 layer		2 layer	
	2.43	4.84	2.40	4.85	2.44	4.84	− 1.62	4.89	− 1.58	4.90	− 1.64	4.89
	3 layer		3 layer		3 layer		4 layer		4 layer		4 layer	
	1.08	4.94	1.21	4.91	1.25	4.90	− 0.92	4.95	− 1.05	4.91	− 1.11	4.91
	5 layer		5 layer		5 layer		6 layer		6 layer		6 layer	
	0.61	4.96	0.92	4.92	0.98	4.91	− 0.56	4.96	− 0.88	4.92	− 0.94	4.91

Table 4
The magnetic moments (M) and the number of d-electrons per atom (N) for Fe_9 cluster and nearest Cr atoms in the presence of the surface

Atom's number in the cluster	Fe_9 touching surface				Fe_9 one layer from the surface			
	FM		AFM		FM		AFM	
	M	N	M	N	M	N	M	N
1	2.45	6.87	− 2.98	6.08	− 2.56	6.79	2.97	6.09
2	2.59	6.61	2.76	6.44	− 2.08	6.67	− 2.18	6.57
3	1.77	6.78	1.84	6.70	− 1.68	6.81	− 1.74	6.74
Cr: 2nd sphere					1 layer		1 layer	
					2.73	4.63	2.74	4.63
	2 layer		2 layer		3 layer		3 layer	
	− 1.65	4.80	− 1.66	4.79	1.35	4.78	1.35	4.79
	4 layer		4 layer		5 layer		5 layer	
	− 1.12	4.79	− 1.12	4.80	1.07	4.79	1.07	4.79
Cr: 3rd sphere					1 layer		1 layer	
					2.38	4.84	2.39	4.84
	2 layer		2 layer		3 layer		3 layer	
	− 1.51	4.91	− 1.51	4.91	1.20	4.91	1.21	4.91
	4 layer		4 layer		5 layer		5 layer	
	− 1.01	4.91	− 1.01	4.91	0.94	4.91	0.94	4.91

For the cluster Fe_2 the magnetic moment of the Fe atoms at the surface layer and at the second layer are equal, 2.13 and -1.90 μ_B, respectively. So, even for subsurface atoms in small clusters the magnetic moments appear to be less than in the bulk α-Fe.

Closely spaced Fe/Cr interface also exerts some influence on the cluster's magnetic structure. Ideal smooth interface of Fe layer have the magnetic moment reduced to 1.75 μ_B. Atoms of successive iron layer have the moments enlarged up to 2.35 μ_B. The Fe clusters touching interface layer make it rough. Some atoms of this layer cease to be the neighbours of Cr ones. As a result, their magnetic moment increases. As for magnetic moments of cluster's atoms, their inner atoms have the enlarged magnetic moment whereas the interface atoms have the diminished moment.

In particular, for the cluster Fe_{15} near the Fe/Cr interface, we obtain the magnetic moments successively away from interface cluster's layers as (4): 2.43 μ_B; (2): 1.94 μ_B; (1): 2.46 μ_B; (5): 1.48 μ_B; (3): 1.89 μ_B; (6): 1.49 μ_B. Numbers in parenthesis means the number of atoms in Fig. 1c. The Cr atoms in the third sphere of the central Fe atom have the magnetic moments -1.51 μ_B, -0.98 μ_B, -0.85 μ_B for the first, third, fifth layer from interface, respectively (instead of -1.20 μ_B, -0.86 μ_B, -0.85 μ_B in the same layers without Fe cluster).

Detailed information about the hybridisation between the electronic states localised on the atoms of Fe cluster and ambient Cr atoms as well as about surface effects can be obtained from the local densities of electronic states (DOS). The DOS of Fe_{15} embedded near the surface (dash line) and far from the surface (solid line) for different self-consistent solutions (FM1 $-$ a, FM2 $-$ b, AFM $-$ c) are shown in Fig. 2. For the cluster implanted in the bulk chromium both ferromagnetic solutions give very close DOS which are similar to the DOS of ferromagnetic iron. AF solution, on the contrary, shows the shape which is more typical for AF chromium [13].

The perturbation caused by the surface existence in the first ferromagnetic solution FM1 appears to be much stronger than in the second solution FM2. Whereas for the FM2 state in Fig. 2b there is only a slight deviation of the dash and solid lines, and for
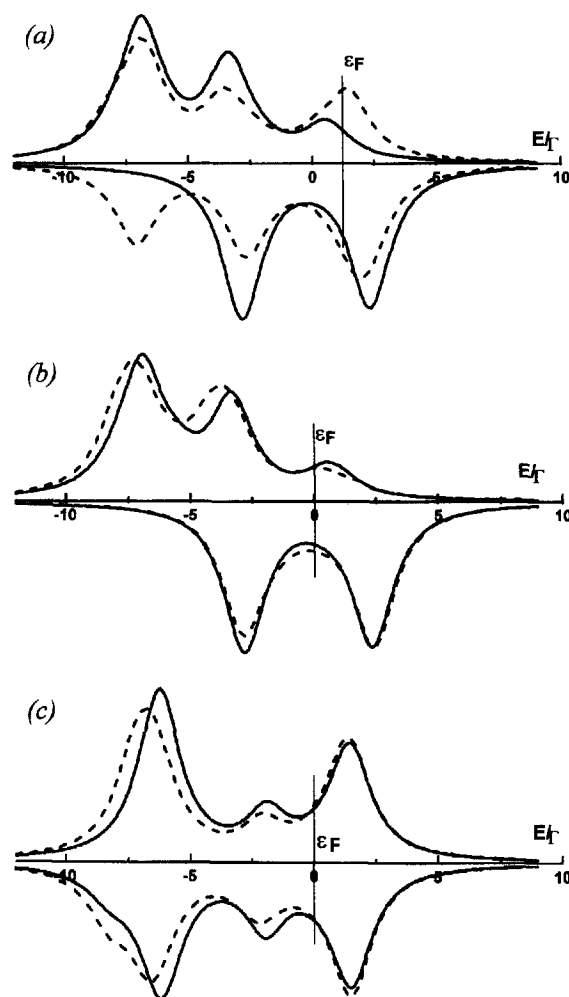

Fig. 2. The density of states (DOS) of Fe_{15} embedded near the surface (dash line) and far from the surface (solid line) for different self-consistent solutions (FM1 – a, FM2 – b, AFM – c).

the FM1 state in Fig. 2a, one can see the transition from FM-type of shape of the DOS toward the AFM-type under the action of surface influence. For the clusters of the smaller size, this influence leads to the transition from the FM structure inside of the cluster to the AFM one.

4. Conclusions

We have calculated the magnetic moments distribution of small Fe clusters embedded in the Cr

matrix near the surface and interface. We have obtained a decrease of magnetic moments for the interface atoms and an increase of the moments for the inner atoms. The surface imposes AF-layered structure on the small Fe cluster. Some of the ferromagnetic solutions which were found for the clusters in the bulk disappear near the surface. The local electronic DOS of embedded Fe clusters reflects clearly the effects of hybridisation and influence of the surface on the magnetic structure. For example, one of ferromagnetic solutions for Fe_{15} changes the shape of DOS under the action of surface proximity so that it becomes more akin to the DOS of AF structure. For the clusters of smaller size the correspondent ferromagnetic solutions can disappear.

Acknowledgements

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